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=> file reg
FILE 'REGISTRY' ENTERED AT 17:00:51 ON 07 MAY 2003
USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.
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=> d his


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L3                STR L2
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L5                SCR 2043 OR 1918
L6             10 S L3 NOT L5
L7                SCR 1611
L8              3 S L3 NOT (L5 OR L7)
L9                SCR 1844
L10             2 S L3 AND L9 NOT (L5 OR L7)
L11            64 S L3 AND L9 NOT (L5 OR L7) FUL
                  SAV L11 YAM589/A

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L12             1 S L11

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L3                STR
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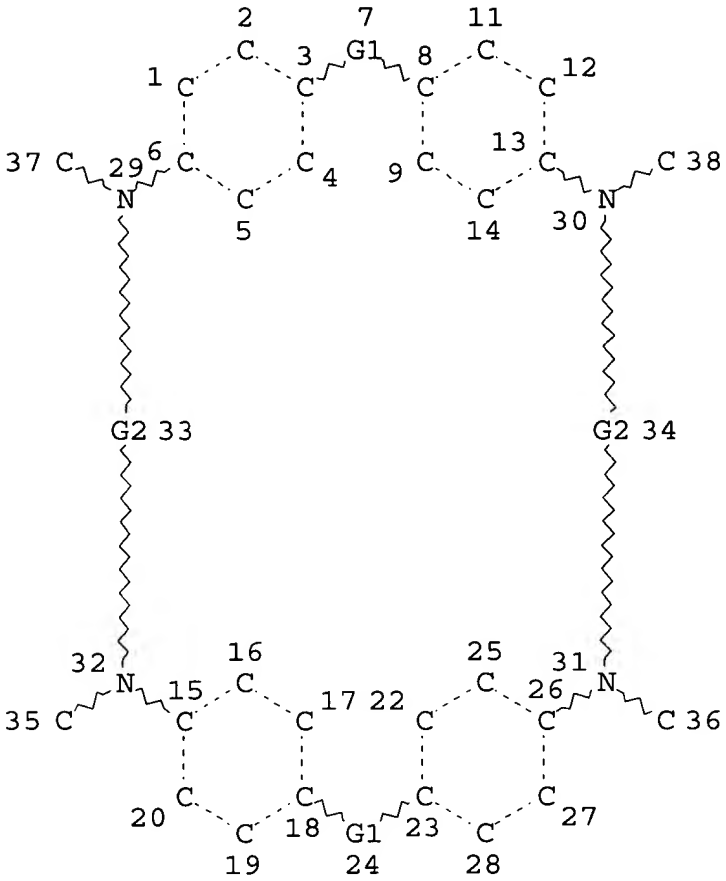

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REP G2=(1-6) A
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DEFAULT MLEVEL IS ATOM
DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:
RING(S) ARE ISOLATED OR EMBEDDED
NUMBER OF NODES IS 36

STEREO ATTRIBUTES: NONE
L5 SCR 2043 OR 1918
L7 SCR 1611
L9 SCR 1844
L11 64 SEA FILE=REGISTRY SSS FUL L3 AND L9 NOT (L5 OR L7)

100.0% PROCESSED 6264 ITERATIONS 64 ANSWERS

SEARCH TIME: 00.00.01

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USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.
PLEASE SEE "HELP USAGETERMS" FOR DETAILS.

FILE COVERS 1907-1966
FILE LAST UPDATED: 01 May 1997 (19970501/UP)

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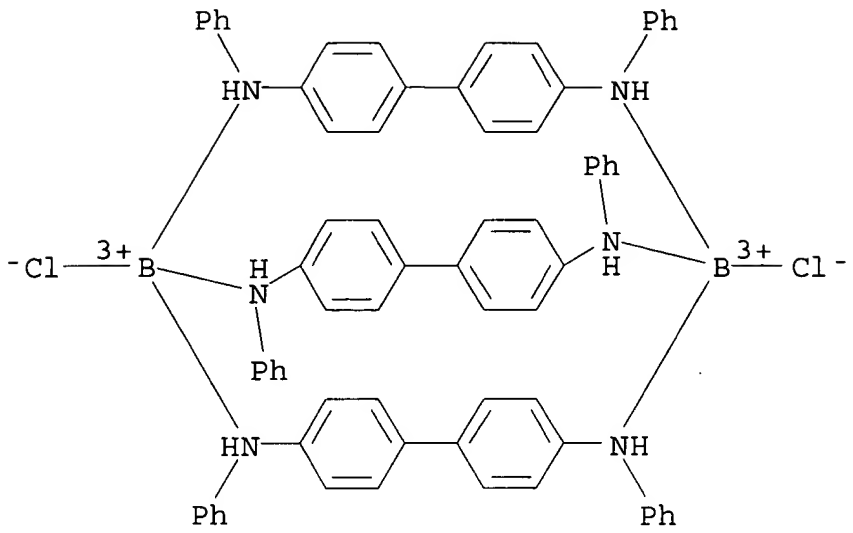
L12 ANSWER 1 OF 1 CAOLD
AN CA64:17023a CAOLD
TI amino derivs. of BCl3
AU Prasad, Sarju; Singh, N. P.
TI polyhedral borane free radicals
AU Lewis, John S.; Kaczmarczyk, A.
IT 7221-02-5 7221-03-6 7221-04-7 7221-05-8 7221-06-9
7221-07-0 **7221-11-6** 7221-12-7 7221-13-8 7240-44-0
7240-45-1 7276-23-5 12447-89-1 12448-36-1
IT **7221-11-6**
RN 7221-11-6 CAOLD
CN Benzidine, N,N'-diphenyl-, compd. with boron chloride (BCl3) (3:2)
(8CI) (CA INDEX NAME)



● 4 Cl⁻

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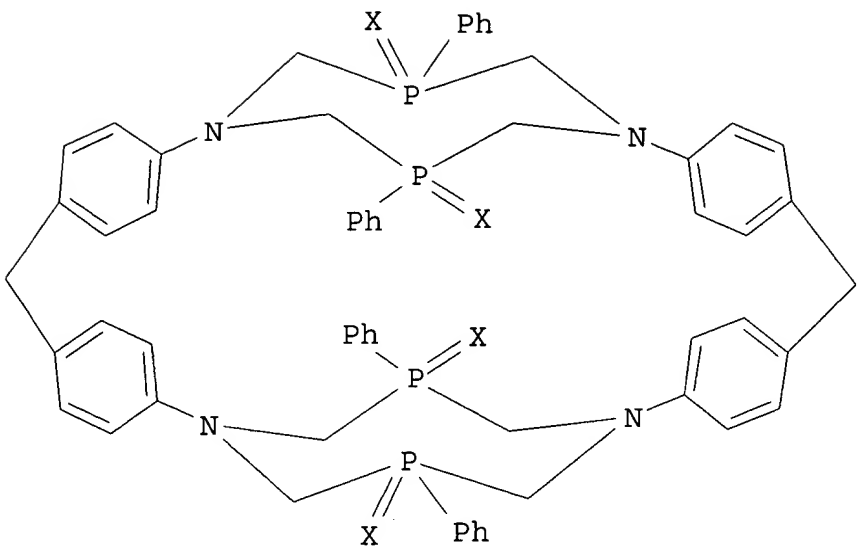
USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.
PLEASE SEE "HELP USAGETERMS" FOR DETAILS.

=> d l13 1-27 cbib abs hitstr hitrn

L13 ANSWER 1 OF 27 ZCA COPYRIGHT 2003 ACS
137:263112 Synthesis of new macrocyclic aminomethylphosphines based on 4,4'-diaminodiphenylmethane and its derivatives. Kuznetsov, R. M.; Balueva, A. S.; Litvinov, I. A.; Gubaidullin, A. T.; Nikonov, G. N.; Karasik, A. A.; Sinyashin, O. G. (A. E. Arbuzov Institute of Organic and Physical Chemistry, Kazan Research Center of the Russian Academy of Sciences, Kazan, 420088, Russia). Russian Chemical Bulletin (Translation of Izvestiya Akademii Nauk, Seriya Khimicheskaya), 51(1), 151-156 (English) 2002. CODEN: RCBUEY. ISSN: 1066-5285. Publisher: Kluwer Academic/Consultants Bureau.
GI



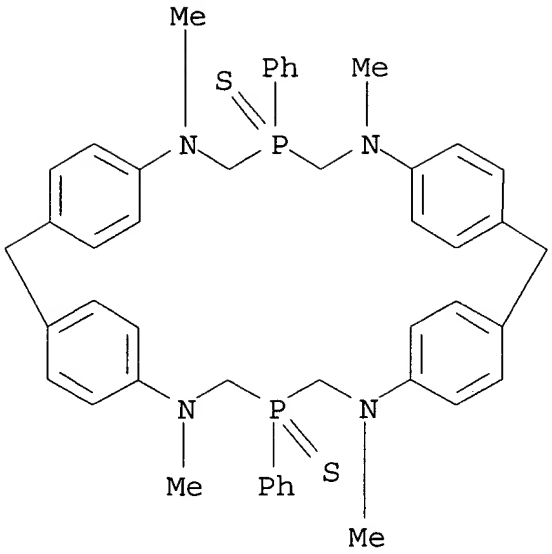
I

AB The reaction of bis(hydroxymethyl)phenylphosphine with 4,4'-diaminodiphenylmethane in DMF afforded bis[methylenedi(p-phenylene)]di(3,7-diphenyl-1,5-diaza-3,7-diphosphacyclooctane) I (X = nothing) whose structure was established by x-ray diffraction anal. Sulfurization and oxidn. of macrocyclic tetraphosphine I gave rise to products I (X = S, O, resp.); compd. I (X = O) being obtained as a stable hexahydrate. The reaction of bis(hydroxymethyl)phenylphosphine with bis(4-N-methylaminophenyl)methane in DMF followed by sulfurization yielded monocyclic bis{methylenedi[p-phenylene(N-methyl)aminomethyl]}di(P-phenyl)phosphine sulfide (4).

IT **462628-76-8P**
(prepn. of)

RN 462628-76-8 ZCA

CN 7,11,21,25-Tetraaza-9,23-diphosphapentacyclo[24.2.2.23,6.212,15.217,20]hexatriaconta-3,5,12,14,17,19,26,28,29,31,33,35-dodecaene, 7,11,21,25-tetramethyl-9,23-diphenyl-, 9,23-disulfide (9CI) (CA INDEX NAME)



IT **462628-76-8P**
(prepn. of)

L13 ANSWER 2 OF 27 ZCA COPYRIGHT 2003 ACS
137:63385 Molecular recognition by wall-assembling-type nanocavity in aqueous media. Ariga, Katsuhiko; Sakai, Daisuke; Ogata, Toshiyuki; Kikuchi, Jun-Ichi (Graduate School of Materials Science, Nara Institute of Science and Technology, Nara, 630-0101, Japan). Journal of Nanoscience and Nanotechnology, 2(1), 41-44 (English) 2002. CODEN: JNNOAR. Publisher: American Scientific Publishers.

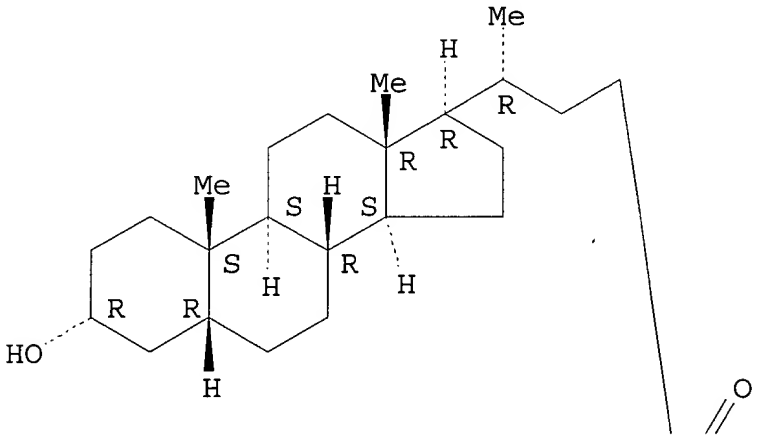
AB Steroid cyclophanes, each having a macrocyclic ring attached to four bile acid moieties via chiral lysine connectors, were synthesized, and the binding of the 2-naphthylphenylketone (guest) to the steroid cyclophanes in water was investigated. The CD spectra of the steroid cyclophane with cholic acid and L-lysine were significantly affected by the binding of the guest, and the induced CD based on the absorption of the achiral guest was also obsd. The binding of the guest to the steroid cyclophane with cholic acids and D-lysines induced changes in the CD spectra with the opposite sign of the mol. ellipticities. An induced CD spectral change was not obsd. upon binding of the guest to the analogous host without OH sites. These results strongly suggest that the guest is conformationally fixed through hydrogen bonding between the carbonyl group of the guest and the steroidal hydroxyl group of the host. The assembly of only four steroid residues on the macrocyclic ring probably provided a hydrophobic nanocavity for hydrogen bonding.

IT **439695-37-1P**
(mol. recognition by steroid cyclophane with lysine connectors)
RN 439695-37-1 ZCA
CN Cholan-24-amide, N,N',N'',N'''-[7,12,22,27-tetraazapentacyclo[26.2.2.23,6.213,16.218,21]octatriaconta-3,5,13,15,18,20,28,30,31,33,35,37-dodecaene-7,12,22,27-

tetrayltetrakis[(1S)-1-(4-aminobutyl)-2-oxo-2,1-ethanediyl]]tetrakis[3-hydroxy-, tetrahydrochloride, (3.alpha.,3'.alpha.,3''.alpha.,3'''.alpha.,5.beta.,5'.beta.,5''.beta.,5'''.beta.)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A



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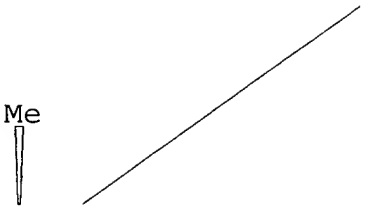

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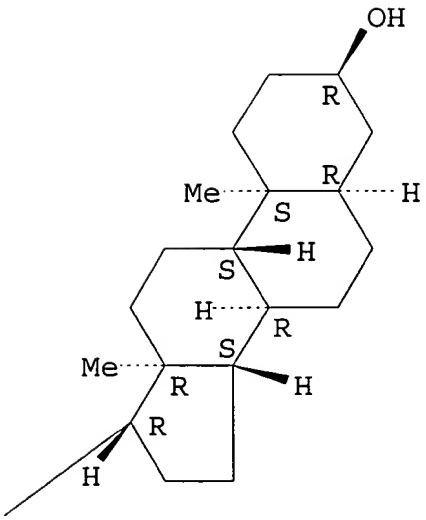

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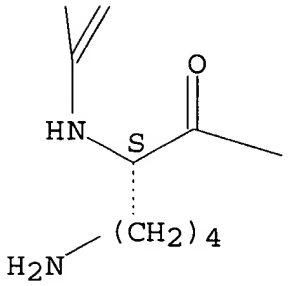

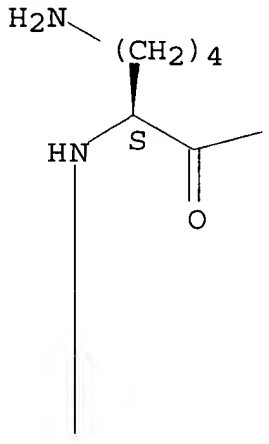

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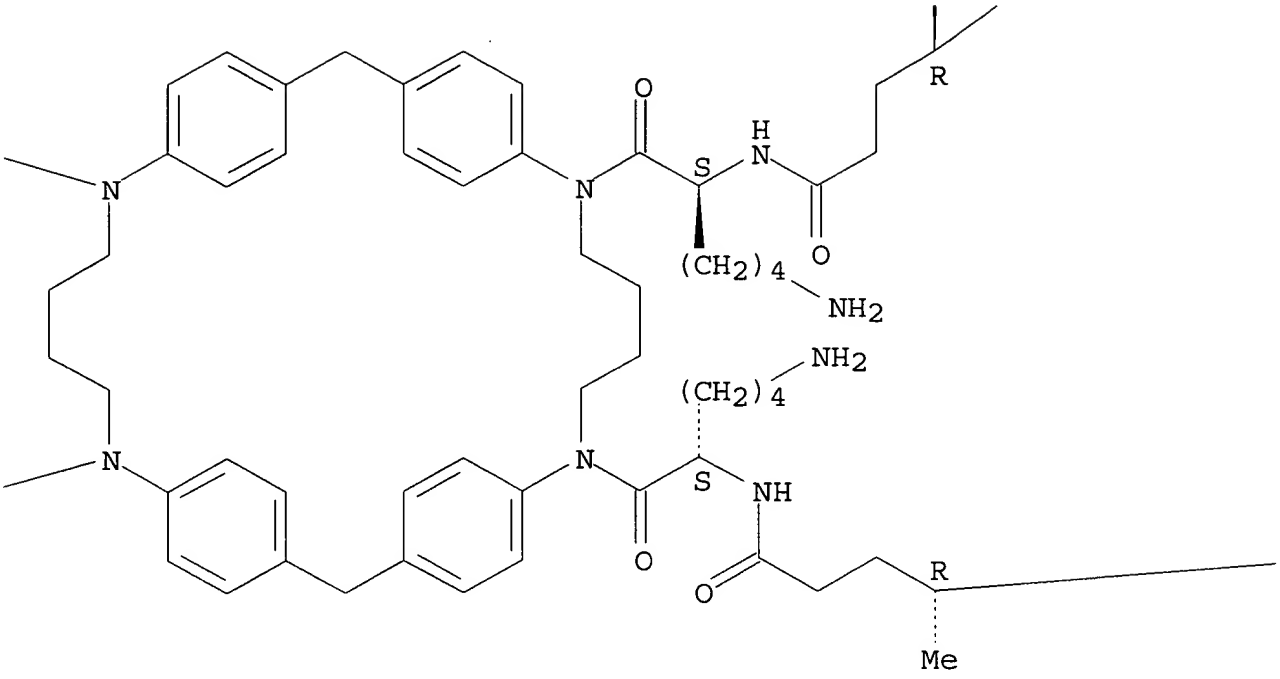

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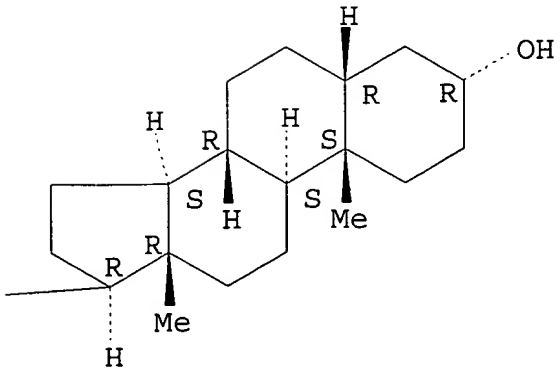

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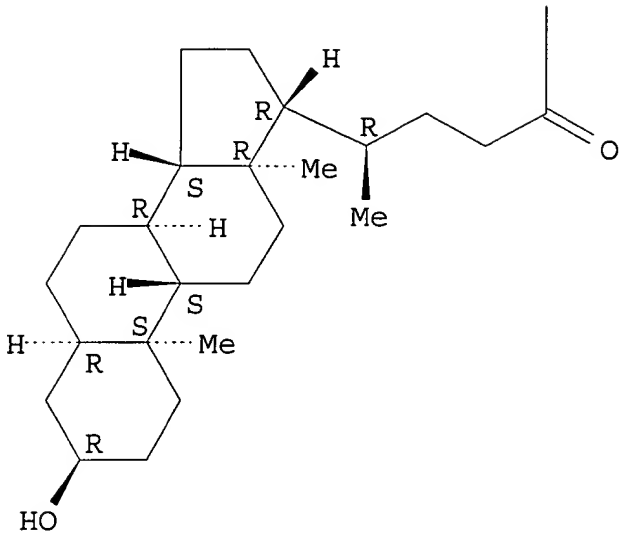
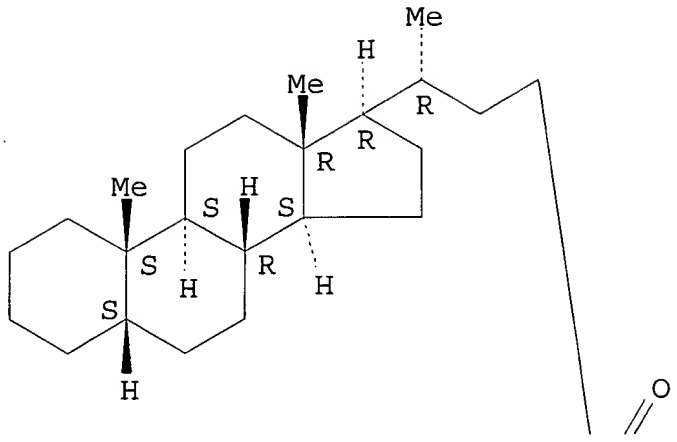


● 4 HCl

IT **439695-38-2P**
(mol. recognition by steroid cyclophane with lysine connectors)
RN 439695-38-2 ZCA
CN Cholan-24-amide, N,N',N'',N'''-[7,12,22,27-tetraazapentacyclo[26.2.2.23,6.213,16.218,21]octatriaconta-3,5,13,15,18,20,28,30,31,33,35,37-dodecaene-7,12,22,27-tetrayltetrakis[(1R)-1-(4-aminobutyl)-2-oxo-2,1-ethanediyl]]tetrakis-, tetrahydrochloride, (5.beta.,5'.beta.,5''.beta.,5'''.beta.)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A



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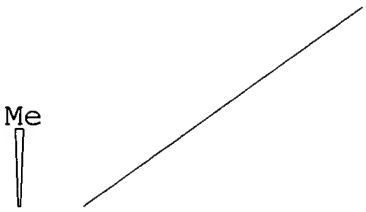

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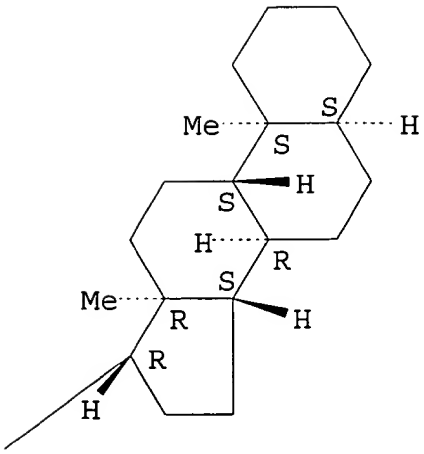

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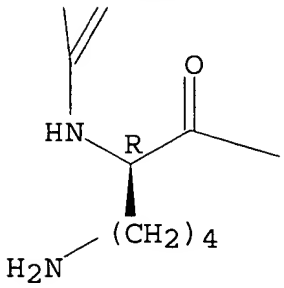

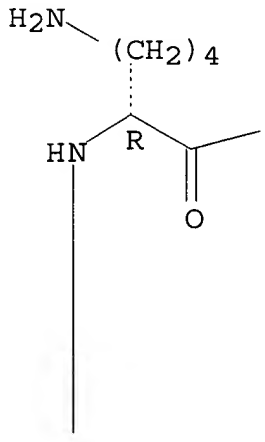

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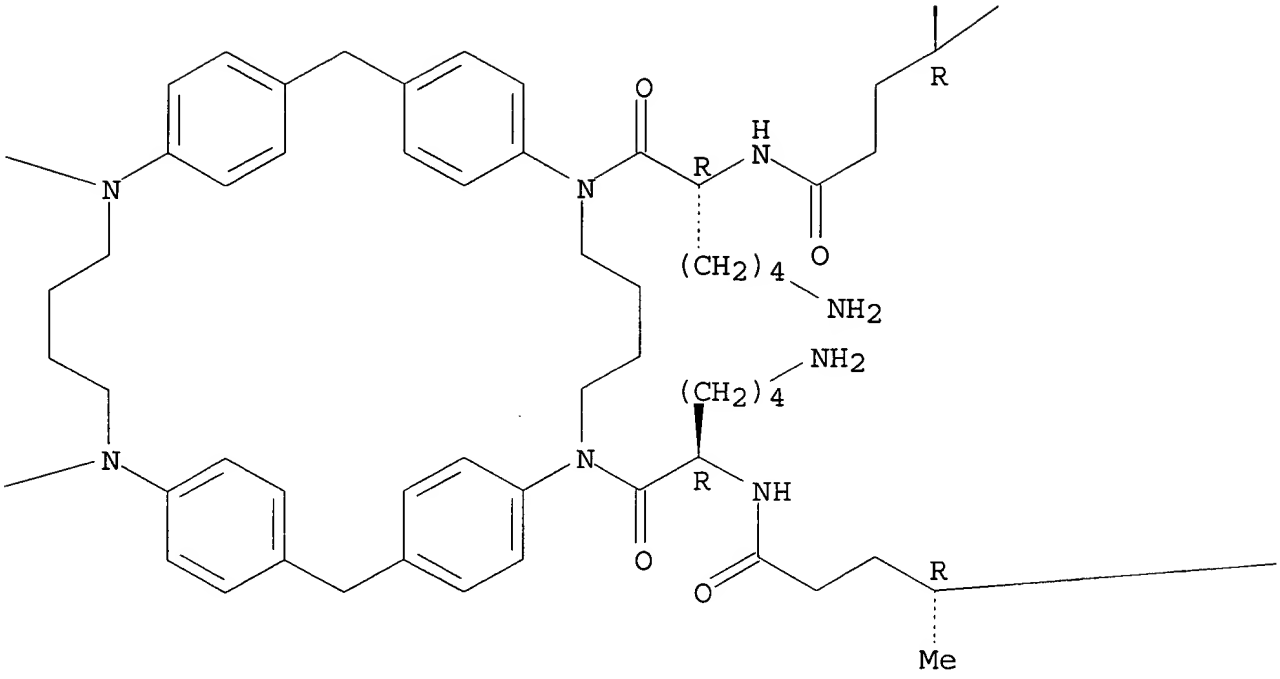

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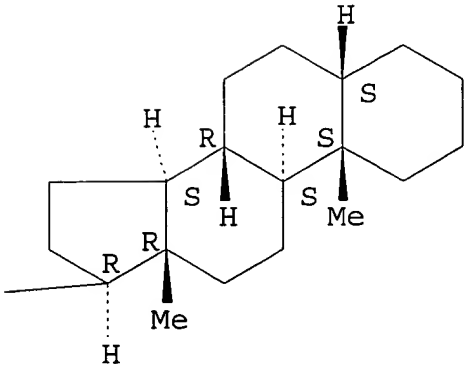

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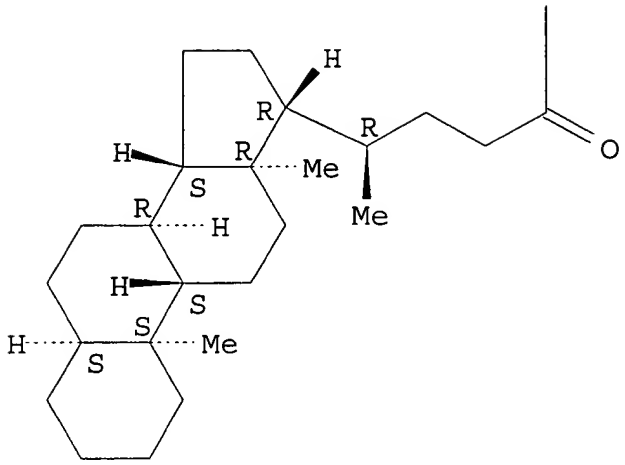
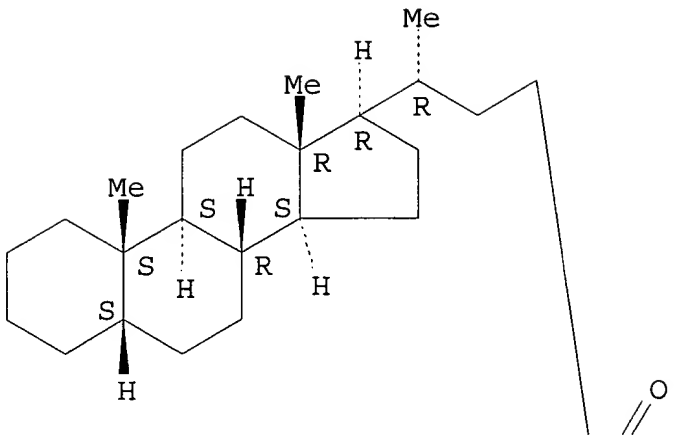


● 4 HCl

IT **351531-44-7P 439695-39-3P**
(mol. recognition by steroid cyclophane with lysine connectors)
RN 351531-44-7 ZCA
CN Cholan-24-amide, N,N',N'',N'''-[7,12,22,27-tetraazapentacyclo[26.2.2.23,6.213,16.218,21]octatriaconta-3,5,13,15,18,20,28,30,31,33,35,37-dodecaene-7,12,22,27-tetrayltetrakis[(1S)-1-(4-aminobutyl)-2-oxo-2,1-ethanediyl]]tetrakis-, tetrahydrochloride (9CI) (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A



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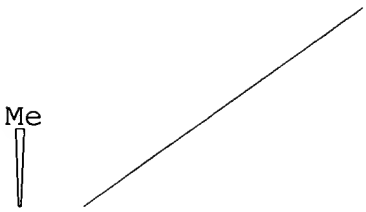

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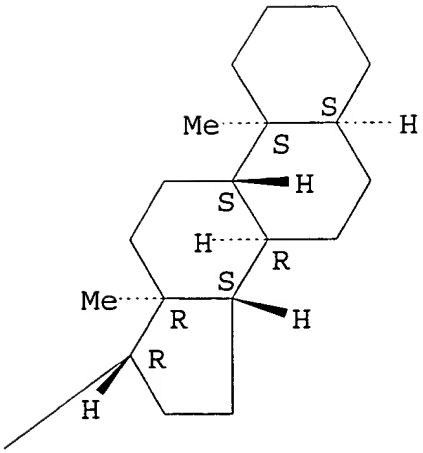

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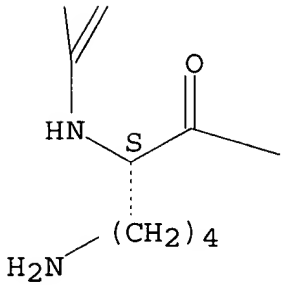

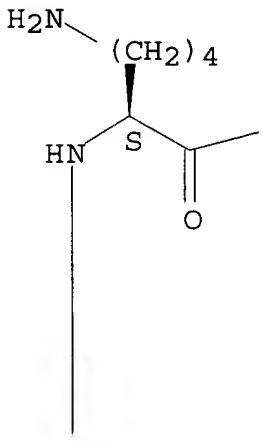

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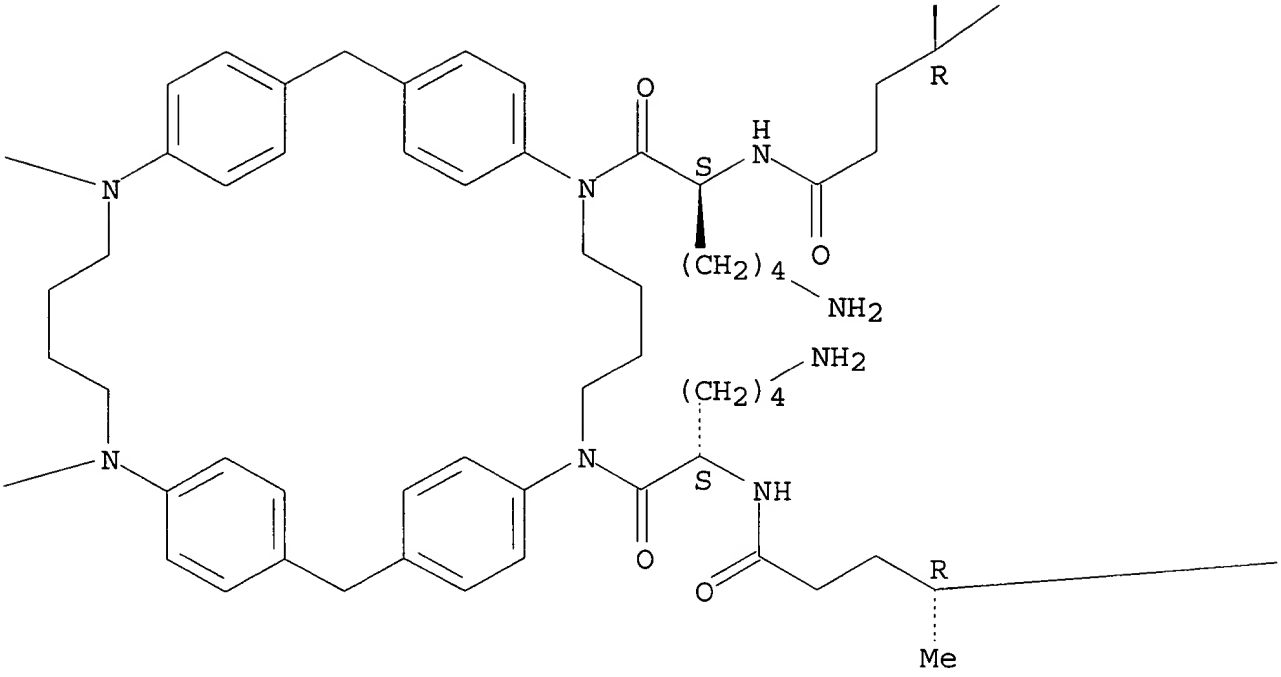

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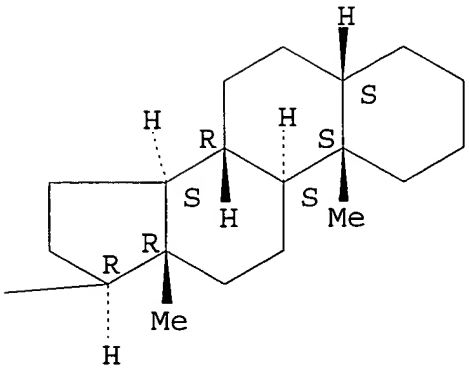

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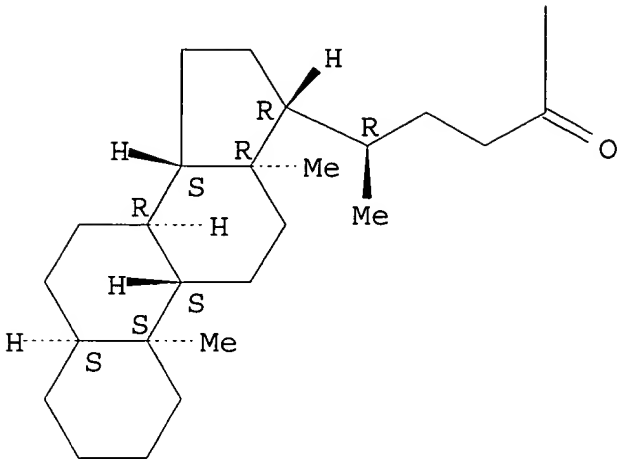

● 4 HCl

RN 439695-39-3 ZCA
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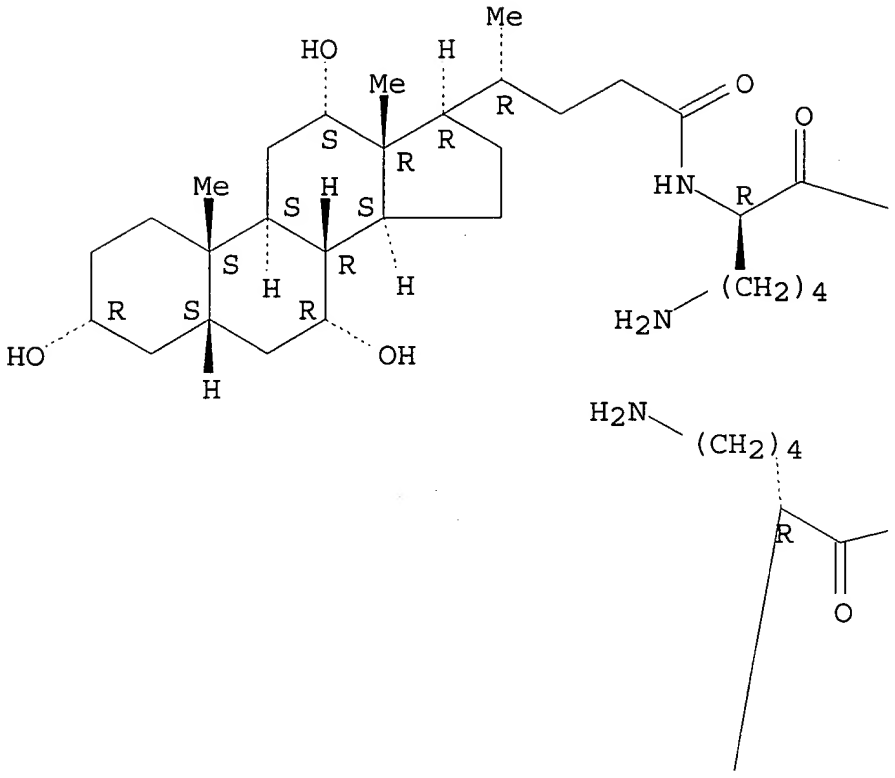
Absolute stereochemistry.

PAGE 1-A



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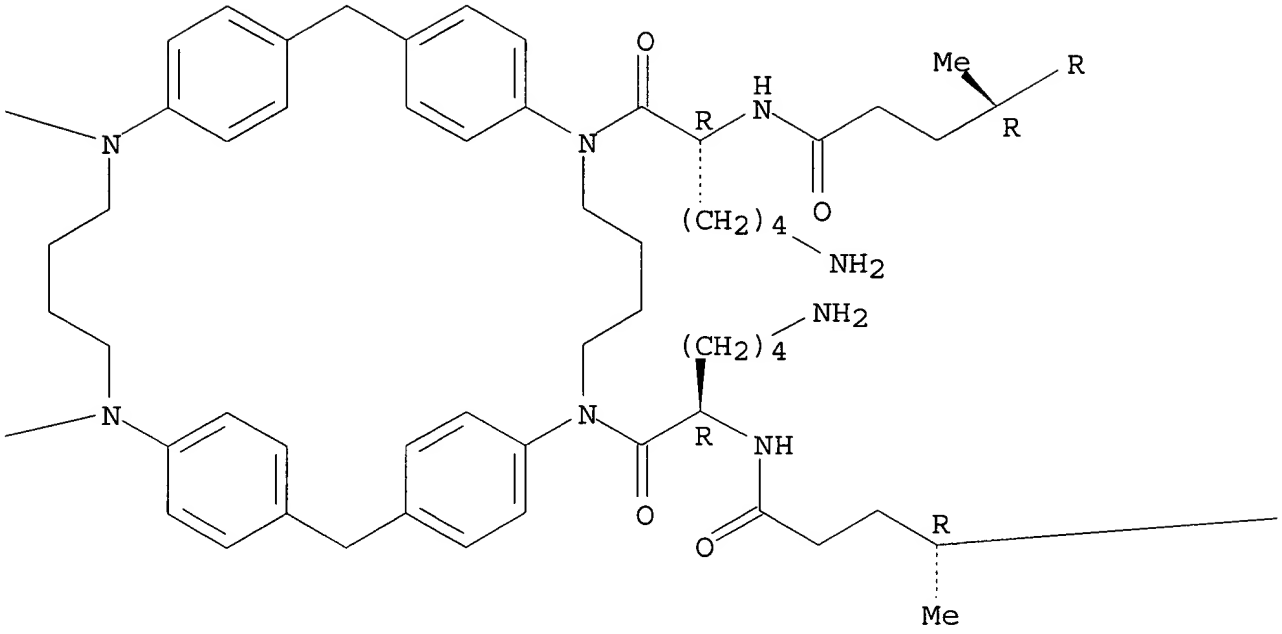

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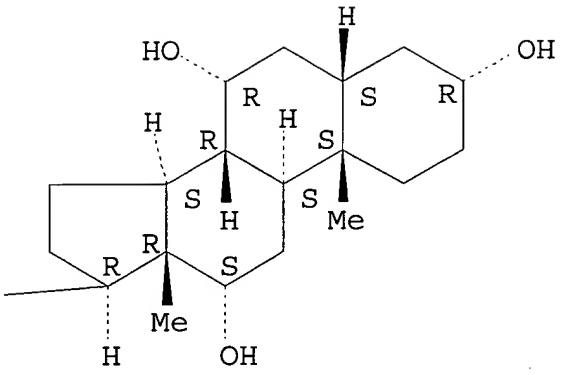

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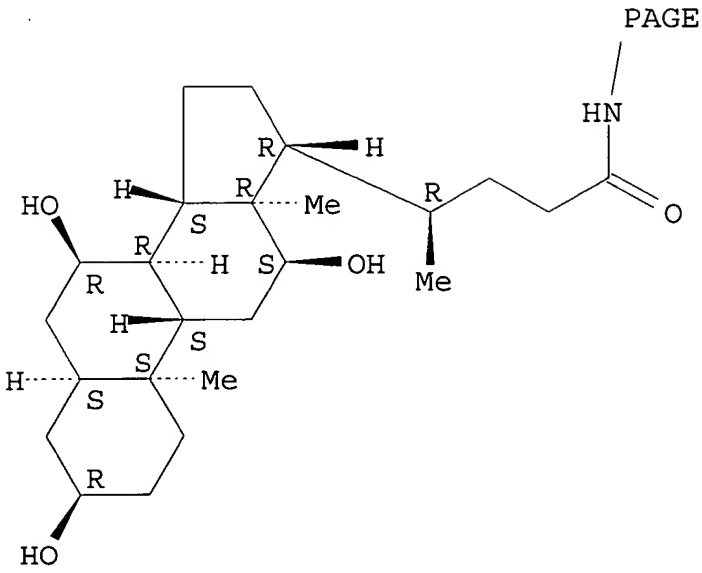

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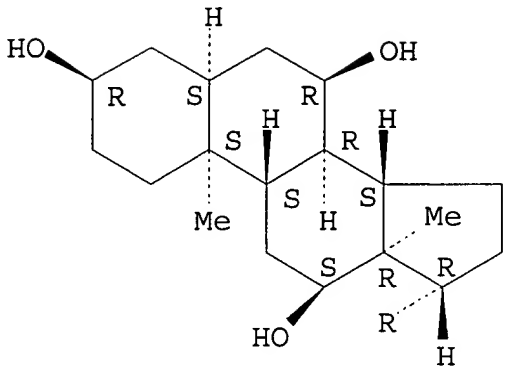

● 4 HCl

IT **156842-46-5**
(mol. recognition by steroid cyclophane with lysine connectors)
RN 156842-46-5 ZCA
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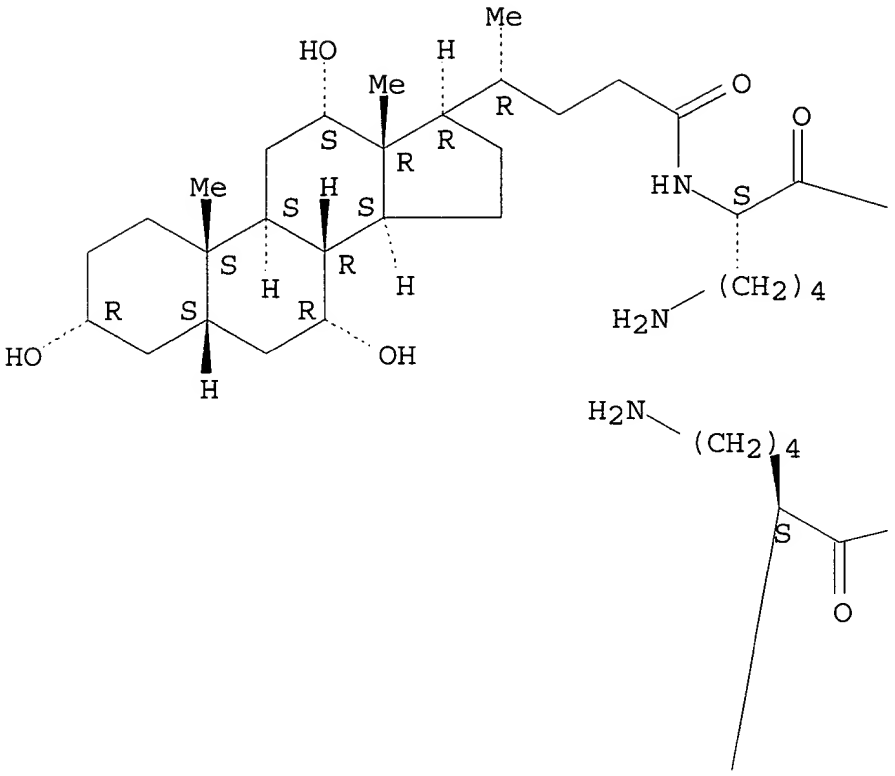
Absolute stereochemistry.

PAGE 1-A



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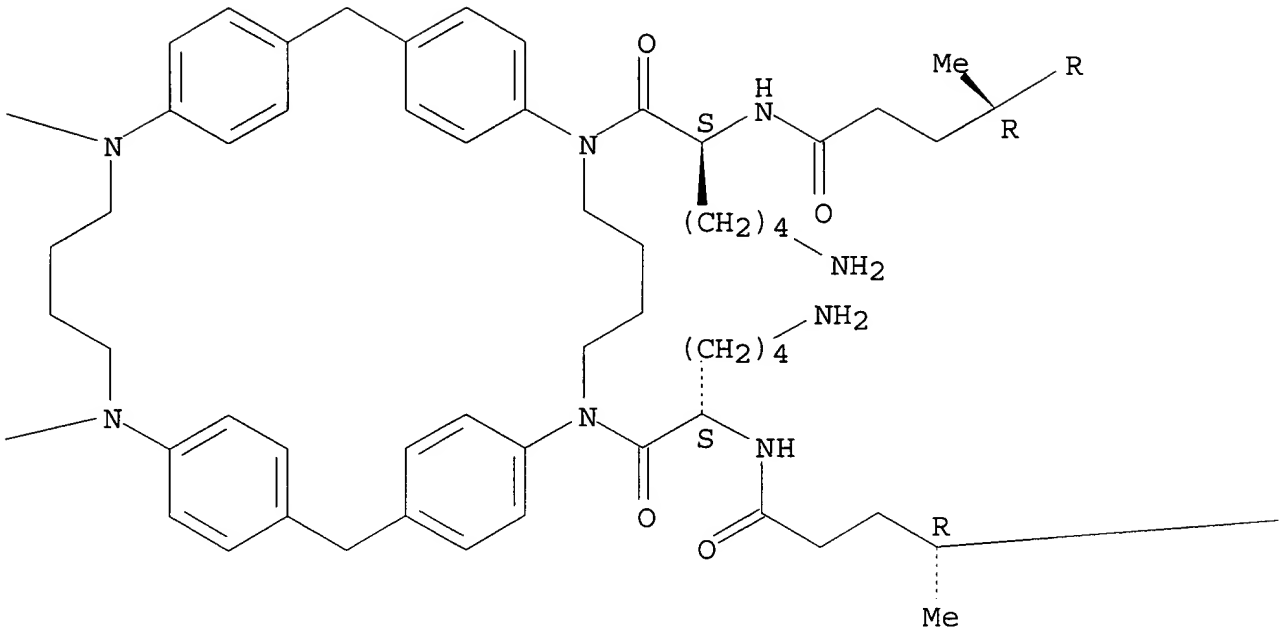

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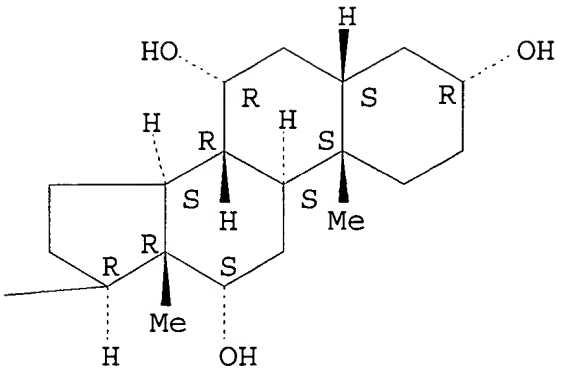
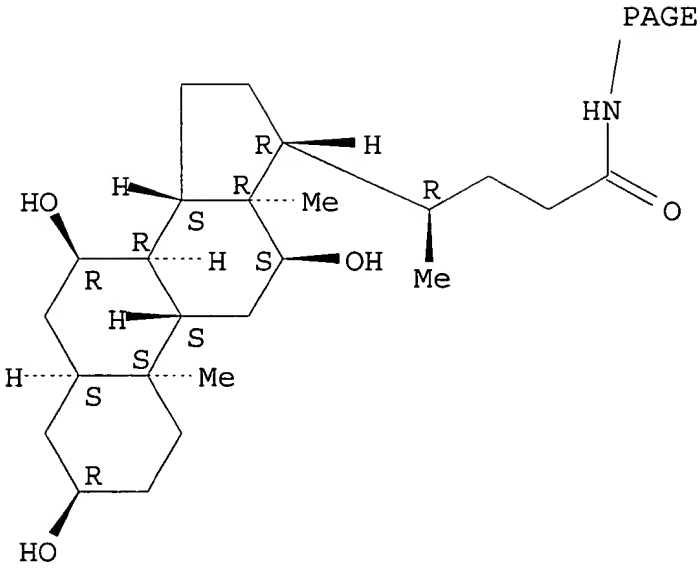


PAGE 2-A



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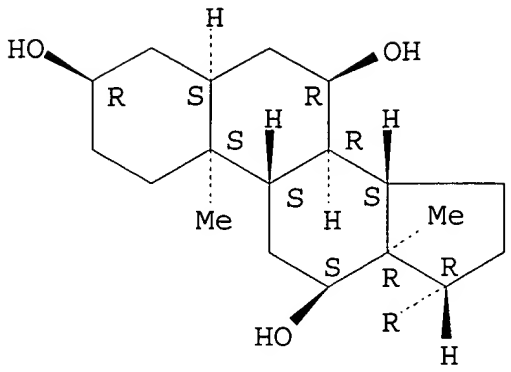


● 4 HCl

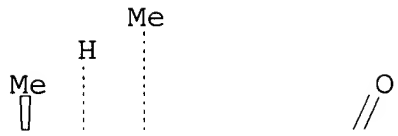
IT **439695-40-6P 439695-41-7P 439695-43-9P**
439695-45-1P
(mol. recognition by steroid cyclophane with lysine connectors)
RN 439695-40-6 ZCA
CN Cholan-24-amide, N,N',N'',N'''-[7,12,22,27-tetraazapentacyclo[26.2.2.23,6.213,16.218,21]octatriaconta-3,5,13,15,18,20,28,30,31,33,35,37-dodecaene-7,12,22,27-tetrayltetrakis[1-(4-aminobutyl)-2-oxo-2,1-ethanediyl]]tetrakis-, stereoisomer, compd. with 2-naphthalenylphenylmethanone (1:1) (9CI) (CA INDEX NAME)

CM 1

CRN 182889-23-2
CMF C154 H240 N12 O8

Absolute stereochemistry.

PAGE 1-A



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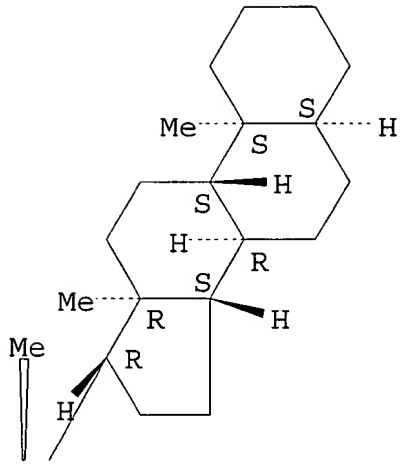

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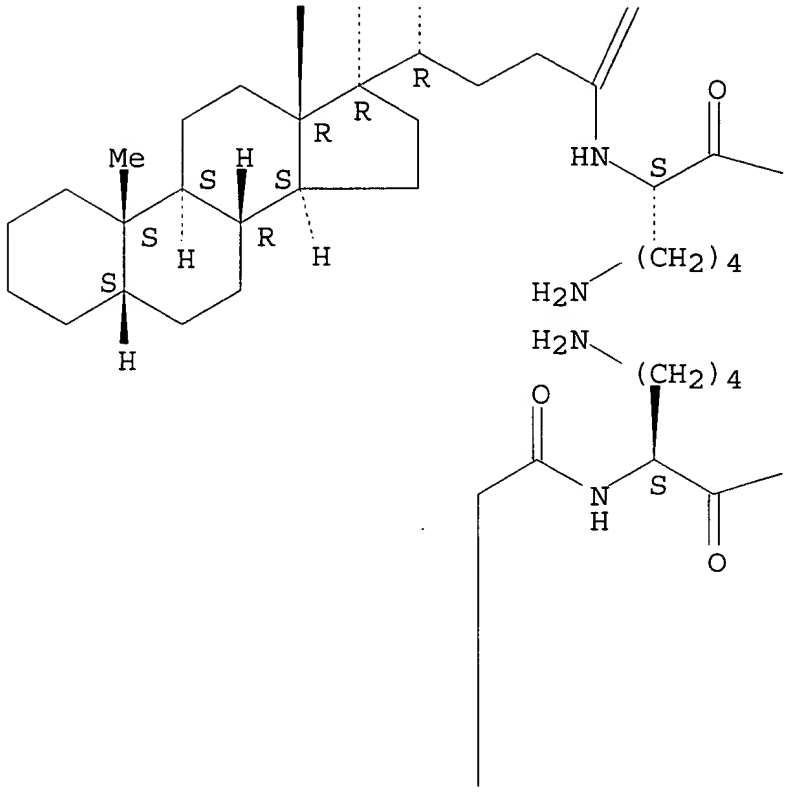

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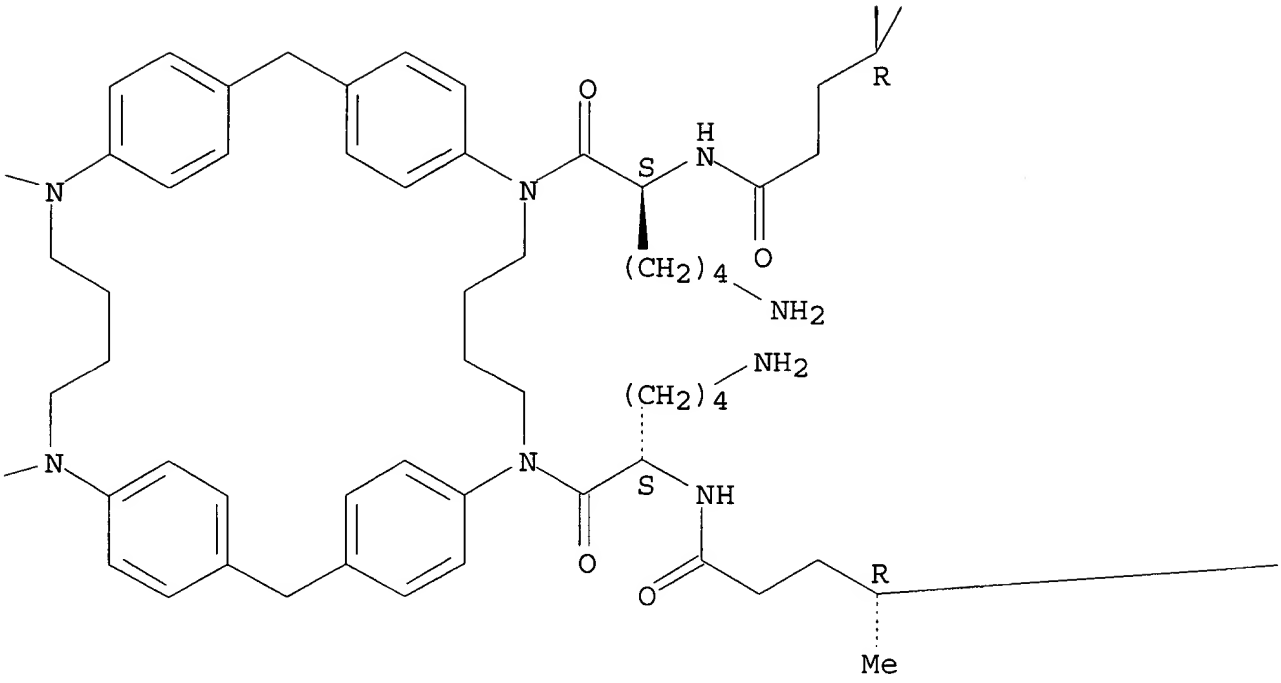
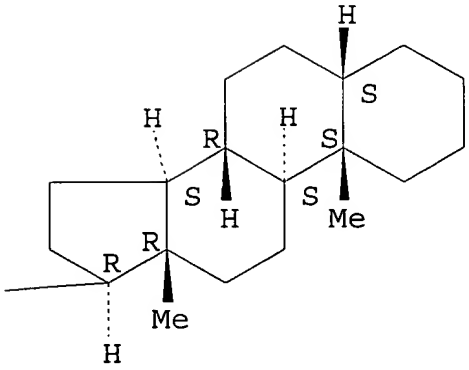


PAGE 2-C



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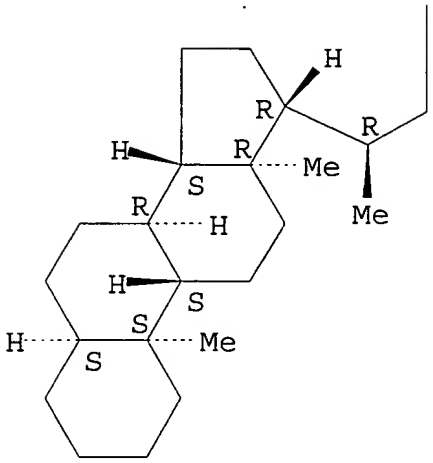
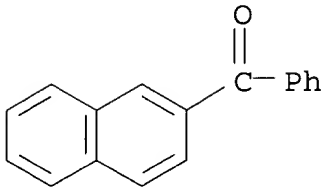


CM 2

CRN 644-13-3
CMF C17 H12 O

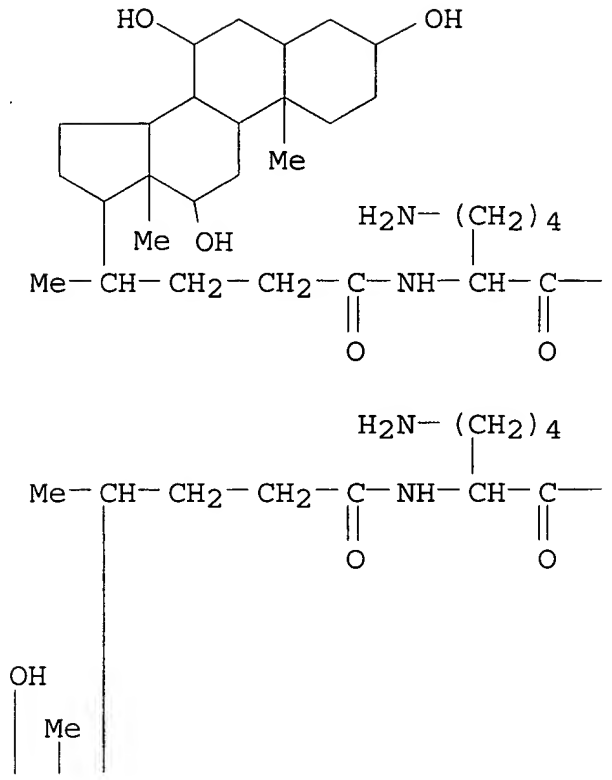


RN 439695-41-7 ZCA
CN Cholan-24-amide, N,N',N'',N'''-[7,12,22,27-tetraazapentacyclo[26.2.2.23,6.213,16.218,21]octatriaconta-3,5,13,15,18,20,28,30,31,33,35,37-dodecaene-7,12,22,27-tetrayltetrakis[1-(4-aminobutyl)-2-oxo-2,1-ethanediyl]]tetrakis[3,7,12-trihydroxy-, stereoisomer, compd. with 2-naphthalenylphenylmethanone (1:1) (9CI) (CA INDEX NAME)

CM 1

CRN 183072-82-4
CMF C154 H240 N12 O20

PAGE 1-A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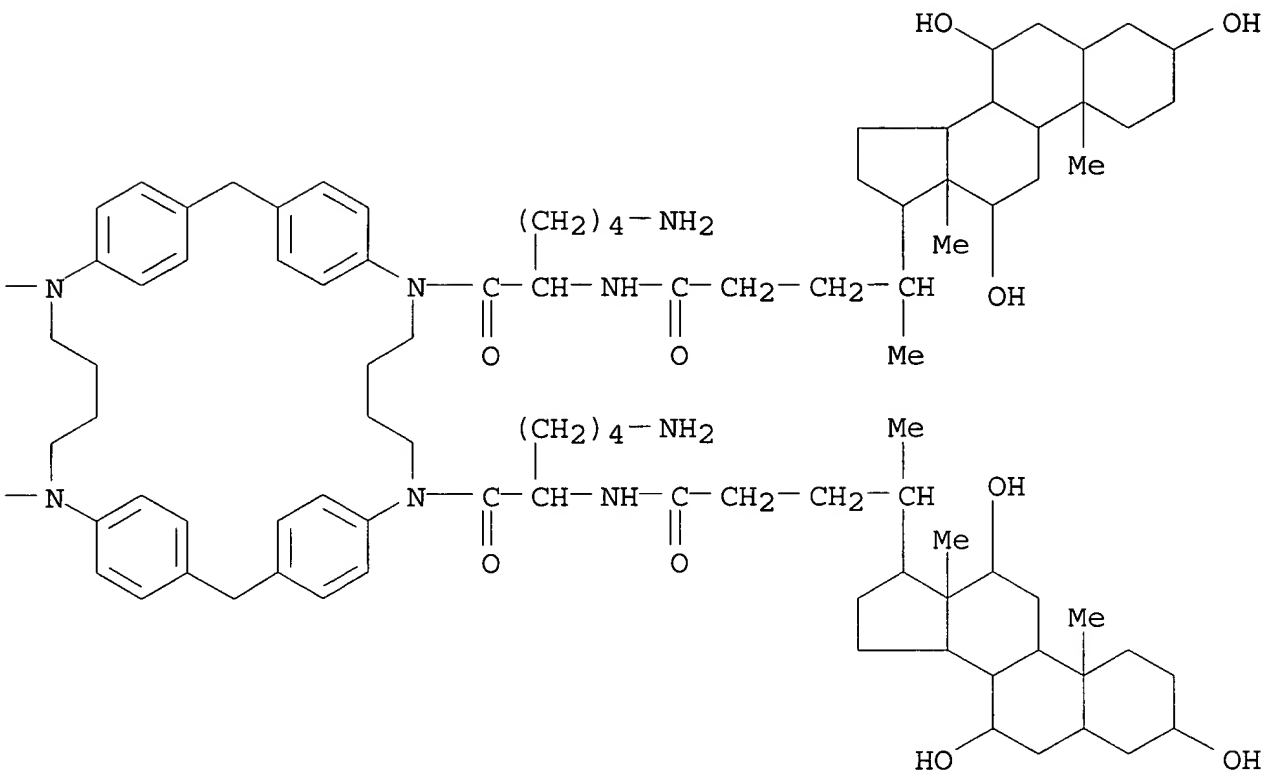
OH
Me
Me
OH
H2N— (CH2)4
Me— CH— CH2— CH2— C— NH— CH— C—
O
O
H2N— (CH2)4
Me— CH— CH2— CH2— C— NH— CH— C—
O
O
OH
Me

PAGE 1-B



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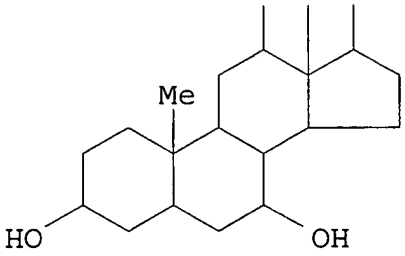
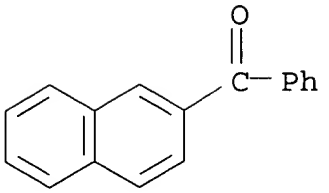


CM 2

CRN 644-13-3
CMF C17 H12 O



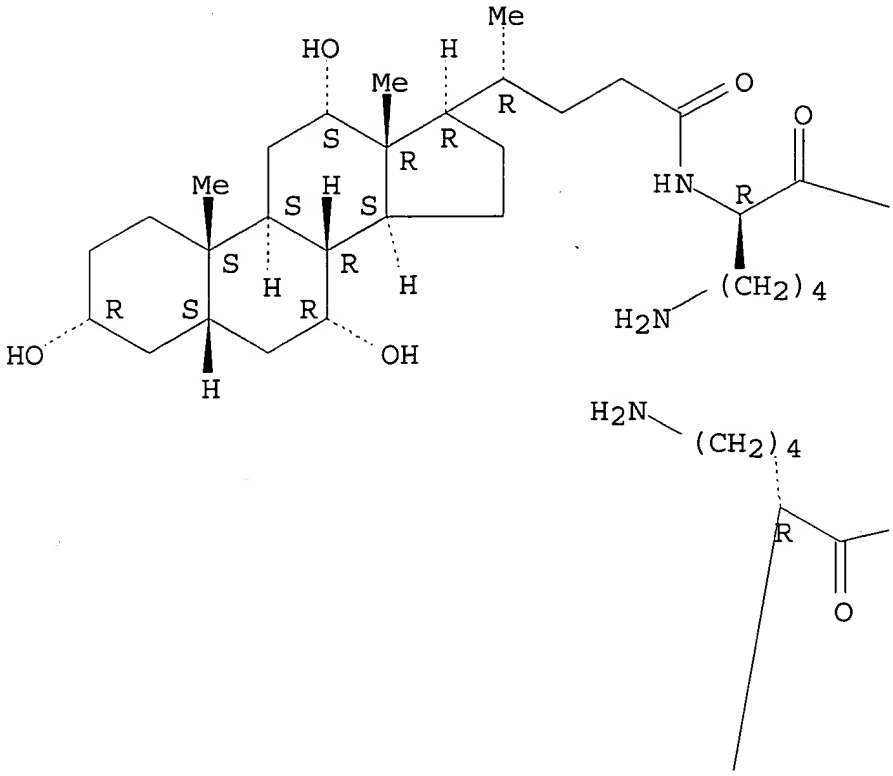
RN 439695-43-9 ZCA
CN Cholan-24-amide, N,N',N'',N'''-[7,12,22,27-tetraazapentacyclo[26.2.2.23,6.213,16.218,21]octatriaconta-3,5,13,15,18,20,28,30,31,33,35,37-dodecaene-7,12,22,27-tetrayltetrakis[1-(4-aminobutyl)-2-oxo-2,1-ethanediyl]]tetrakis[3,7,12-trihydroxy-, (3.alpha.,5.beta.,7.alpha.,12.alpha.)-(3'.alpha.,5'.beta.,7'.alpha.,12'.alpha.)-(3''.alpha.,5''.beta.,7''.alpha.,12''.alpha.)-(3'''.alpha.,5'''.beta.,7'''.alpha.,12'''.alpha.)-, compd. with 2-naphthalenylphenylmethanone (1:1) (9CI) (CA INDEX NAME)

CM 1

CRN 439695-42-8
CMF C154 H240 N12 O20

Absolute stereochemistry.

PAGE 1-A



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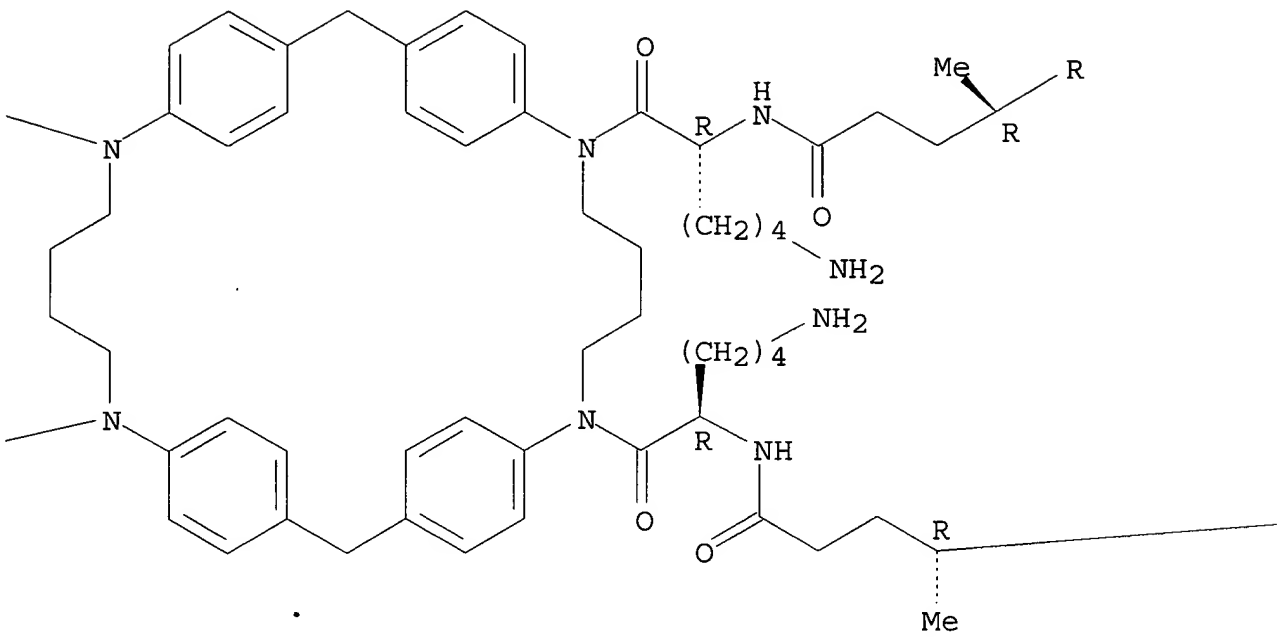

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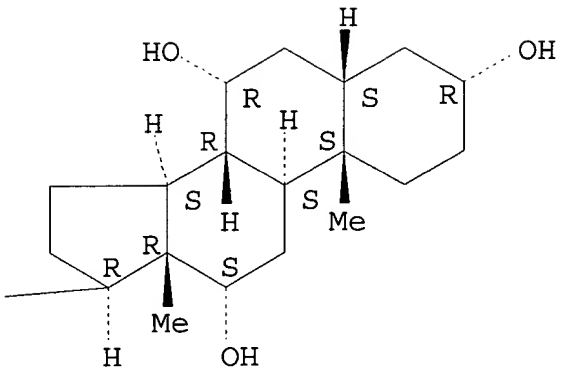

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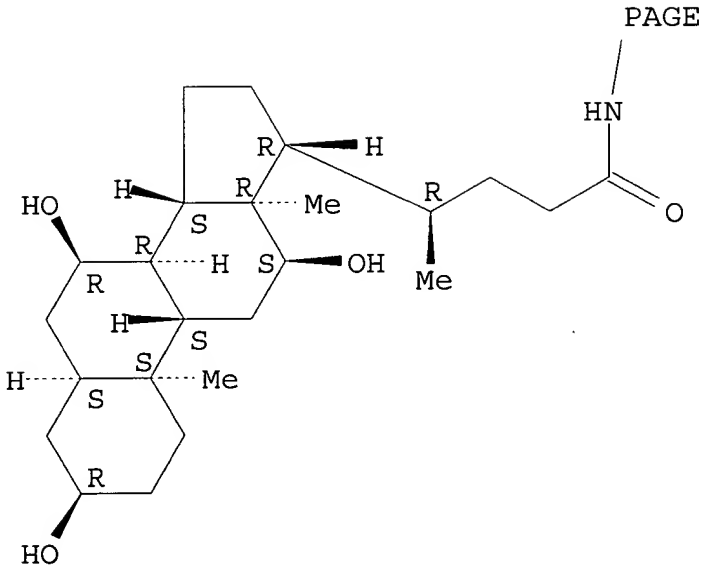

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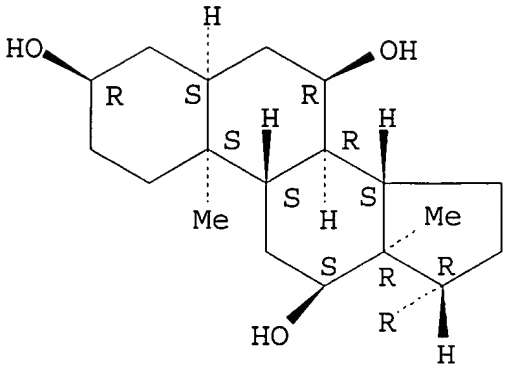
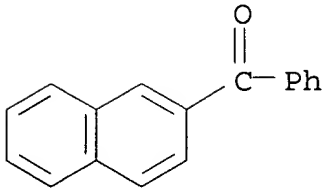


CM 2

CRN 644-13-3
CMF C17 H12 O



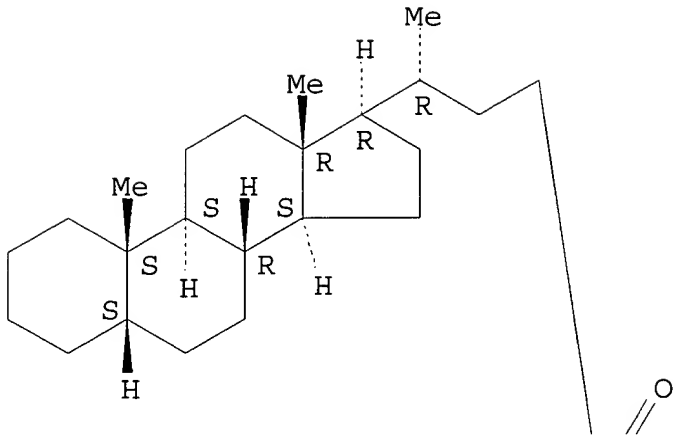
RN 439695-45-1 ZCA
CN Cholan-24-amide, N,N',N'',N'''-[7,12,22,27-tetraazapentacyclo[26.2.2.23,6.213,16.218,21]octatriaconta-3,5,13,15,18,20,28,30,31,33,35,37-dodecaene-7,12,22,27-tetrayltetrakis[1-(4-aminobutyl)-2-oxo-2,1-ethanediyl]]tetrakis-, (5.beta.)-(5'.beta.)-(5''.beta.)-(5'''.beta..alpha.)-, compd. with 2-naphthalenylphenylmethanone (1:1) (9CI) (CA INDEX NAME)

CM 1

CRN 439695-44-0
CMF C154 H240 N12 O8

Absolute stereochemistry.

PAGE 1-A



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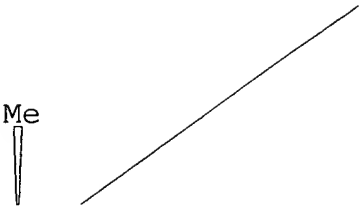

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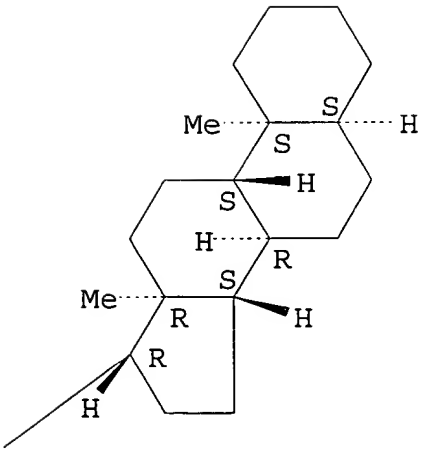

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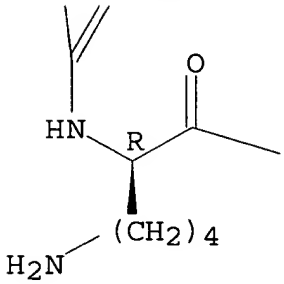

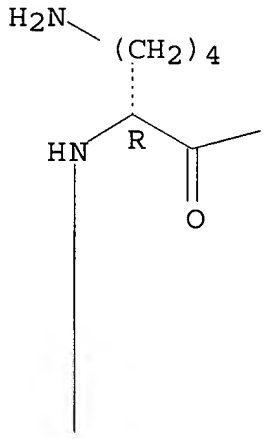

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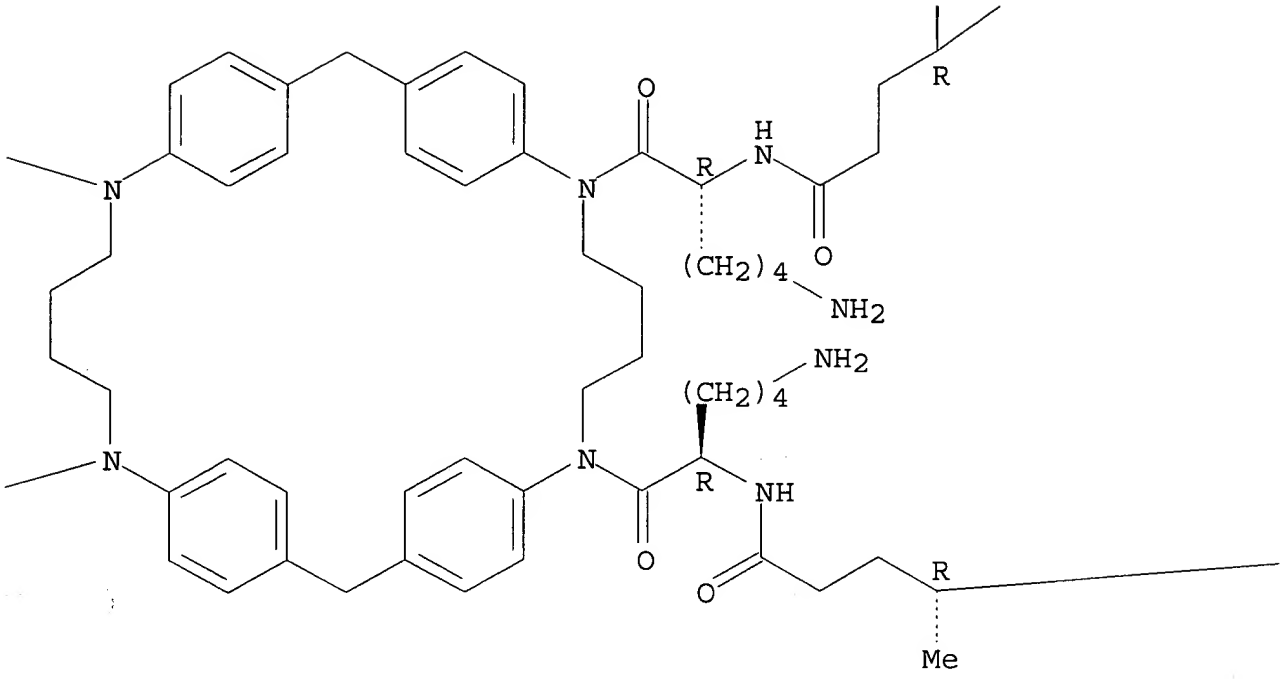

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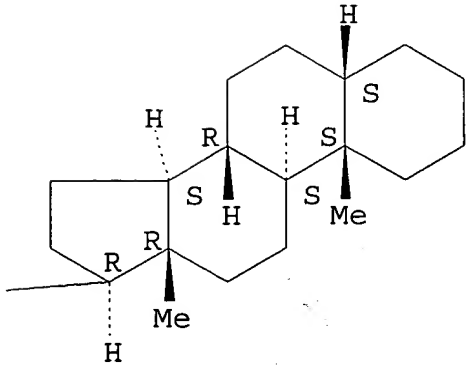
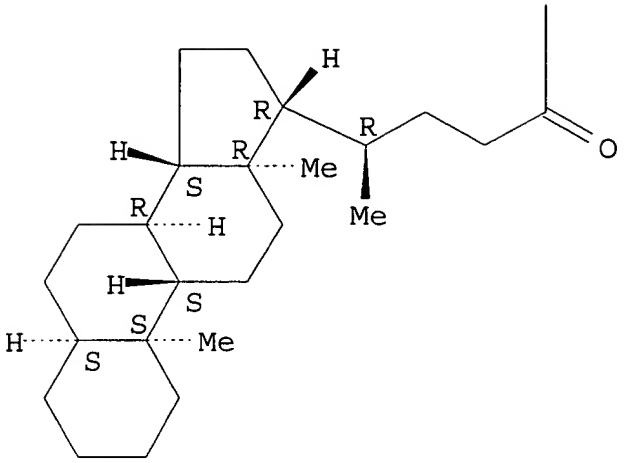
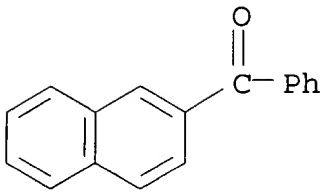


PAGE 3-A



CM 2

CRN 644-13-3
CMF C17 H12 O



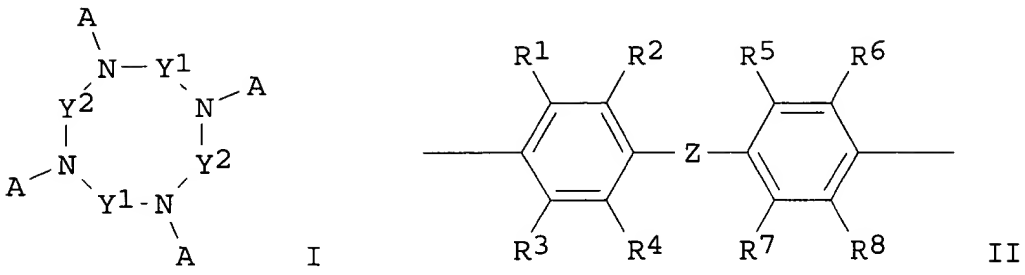
IT **439695-37-1P**
(mol. recognition by steroid cyclophane with lysine connectors)
IT **439695-38-2P**
(mol. recognition by steroid cyclophane with lysine connectors)
IT **351531-44-7P 439695-39-3P**
(mol. recognition by steroid cyclophane with lysine connectors)
IT **156842-46-5**
(mol. recognition by steroid cyclophane with lysine connectors)
IT **439695-40-6P 439695-41-7P 439695-43-9P**
439695-45-1P
(mol. recognition by steroid cyclophane with lysine connectors)

L13 ANSWER 3 OF 27 ZCA COPYRIGHT 2003 ACS
136:377223 Cyclic tertiary amines and organic electroluminescent devices employing the amines as a hole-transporting material, a hole-injecting material or a light-emitting material. Wang, Guofang; Uchida, Manabu; Yokoi, Hajime; Nakano, Takaharu; Furukawa, Kenji (Japan). U.S. Pat. Appl. Publ. US 20020058155 A1 20020516, 12 pp. (English). CODEN: USXXCO. APPLICATION: US 2001-965589 20010926. PRIORITY: JP 2000-297209 20000928; JP 2001-193511

present app

20010626.

GI

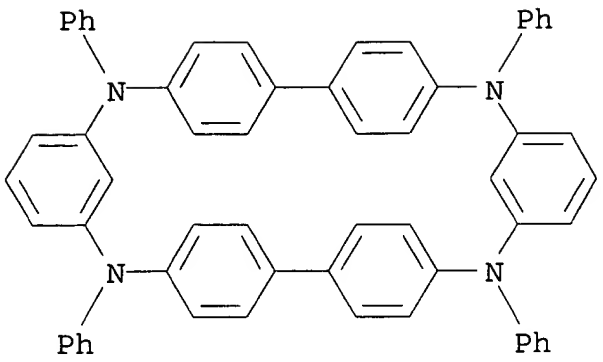


AB Cyclic tertiary amine compds. are described by the formula I, where A = an alkyl group with 1-6 C atoms, a substituted or unsubstituted aryl group, a substituted or unsubstituted aralkyl group, or a substituted or unsubstituted heterocyclic group, and the 4 A substituents may be the same or partly different; Y1 = a substituted or unsubstituted arylene group, or a substituted or unsubstituted heterocyclic divalent group; Y2 = group with formula II, a substituted or unsubstituted condensed ring arylene group, or a substituted or unsubstituted heterocyclic divalent group, where R1-8 independently represents H, a halogen atom, an alkyl or alkoxy group having 1-6 C atoms, an aryl group or a heterocyclic group; and Z represents single bond, an arylene group, -CH2-, -CH=CH-, -C.ident.C-, -C(CH3)2-, -CO-, -O-, -S- or -SO2-. Org. electroluminescent devices employing the cyclic tertiary amines as a hole transport material, a hole injection material or a light-emitting material are also described and show a high luminous efficiency and a long service life.

IT **425369-05-7P**
(cyclic tertiary amines and org. electroluminescent devices employing amines as hole-transporting material, hole-injecting material or light-emitting material)

RN 425369-05-7 ZCA

CN 6,12,21,27-Tetraazaheptacyclo[26.2.2.22,5.213,16.217,20.17,11.122,26]tetraconta-2,4,7,9,11(38),13,15,17,19,22,24,26(33),28,30,31,34,36,39-octadecaene, 6,12,21,27-tetraphenyl- (9CI) (CA INDEX NAME)



IT **425369-05-7P**
(cyclic tertiary amines and org. electroluminescent devices employing amines as hole-transporting material, hole-injecting material or light-emitting material)

L13 ANSWER 4 OF 27 ZCA COPYRIGHT 2003 ACS
136:191008 Modulation of photo-signal based on molecular recognition by steroid cyclophane in liquid assembly. Ariga, Katsuhiko; Sakai, Daisuke; Terasaka, Yukiko; Kikuchi, Jun-Ichi (Graduate School of Materials Science, Nara Institute of Science and Technology, Nara, 630-0101, Japan). Molecular Crystals and Liquid Crystals Science and Technology, Section A: Molecular Crystals and Liquid Crystals, 370, 343-346 (English) 2001. CODEN: MCLCE9. ISSN: 1058-725X. Publisher: Gordon & Breach Science Publishers.

AB The binding of a fluorescent probe (TNS) in aq. mixts. of a steroid cyclophane and an artificial lipid was spectrophotometrically studied. When the content of the steroid cyclophane is dominant ([lipid]/[cyclophane] = 0.1), the fluorescent max. of the bound TNS is 433 nm. At the [lipid]/[cyclophane] ratio of 5, the fluorescence max. is .apprx.409 nm, indicating that the host cavity provided a more hydrophobic environment. A large excess of lipid reversed the fluorescence max. up to 426 nm, i.e., the host cavity became hydrophilic again. The change in emission maxima of the bound TNS is modulated by the hydrophobic-hydrophilic cavity conversion.

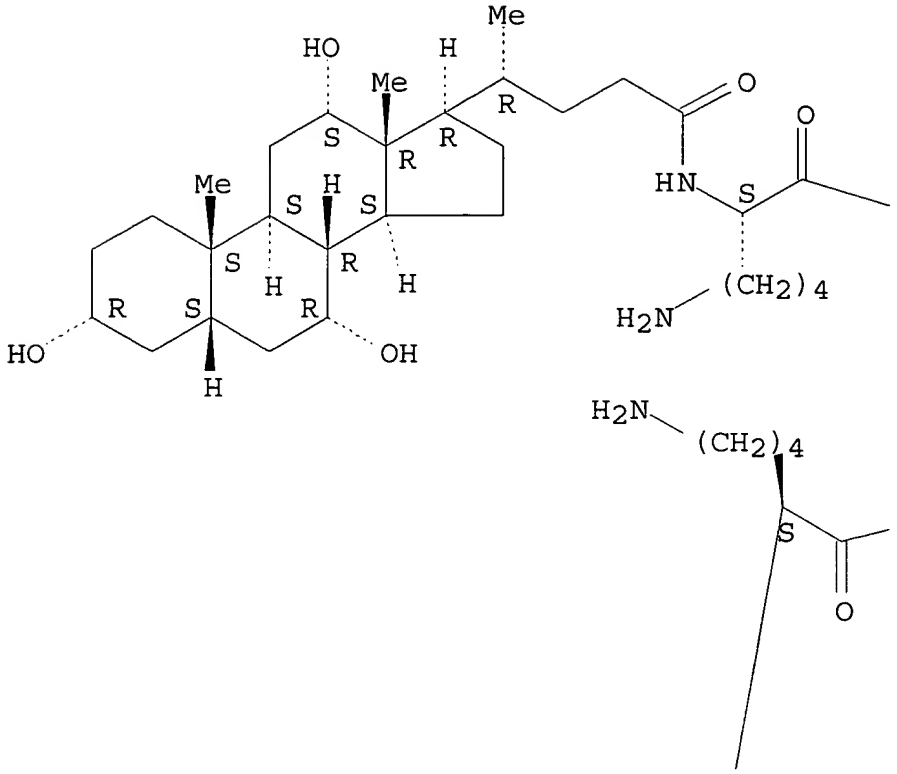
IT **156842-46-5 351531-44-7**
(modulation of photo-signal based on mol. recognition by steroid cyclophane in liq. assembly)

RN 156842-46-5 ZCA

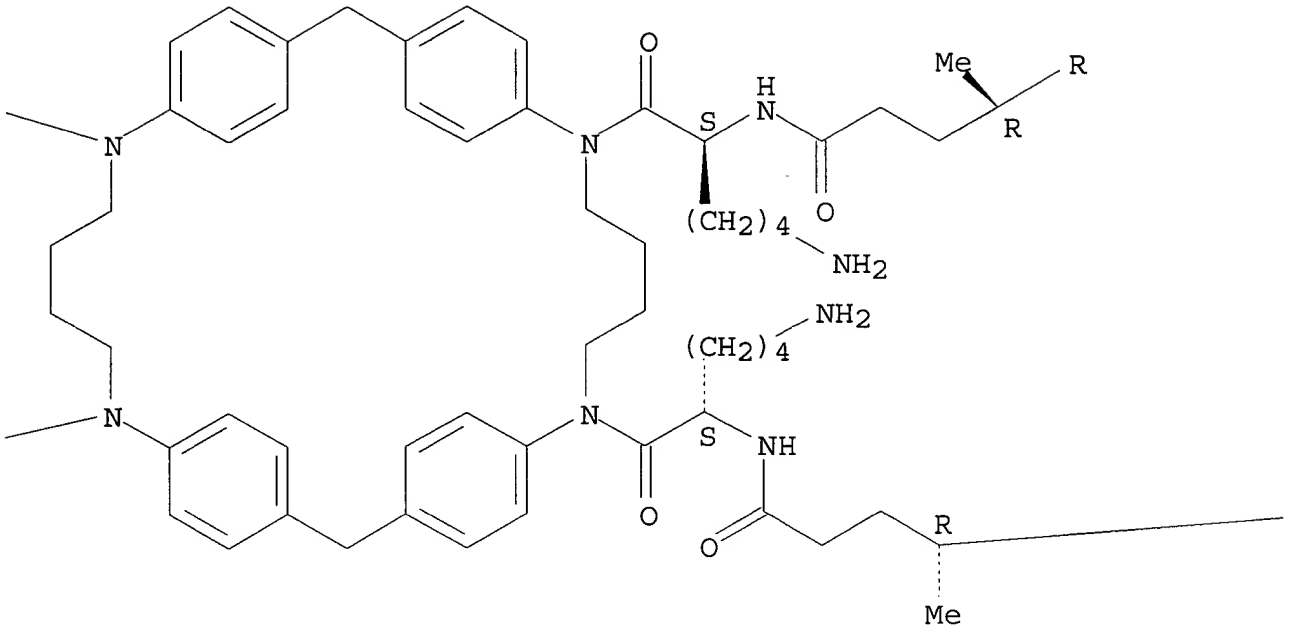
CN Cholan-24-amide, N,N',N'',N'''-[7,12,22,27-tetraazapentacyclo[26.2.2.23,6.213,16.218,21]octatriaconta-3,5,13,15,18,20,28,30,31,33,35,37-dodecaene-7,12,22,27-tetrayltetrakis[1-(4-aminobutyl)-2-oxo-2,1-ethanediyl]]tetrakis[3,7,12-trihydroxy-, tetrahydrochloride, stereoisomer (9CI) (CA INDEX NAME)

Absolute stereochemistry.

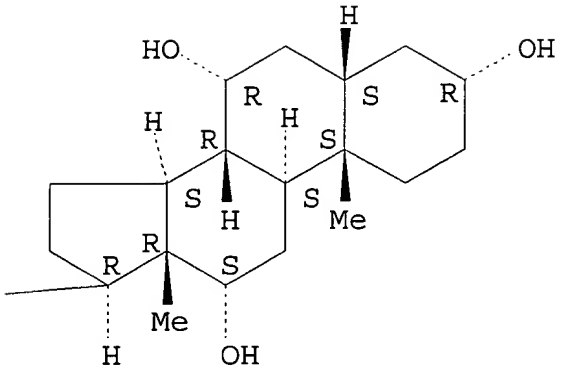
PAGE 1-A


Me
HO
H
Me
O
R
S
R
R
O
HN
S
Me
S
H
S
H
S
R
H
(CH2)4
H2N
R
S
H
R
H
HO
OH
H
H2N
(CH2)4
S
O

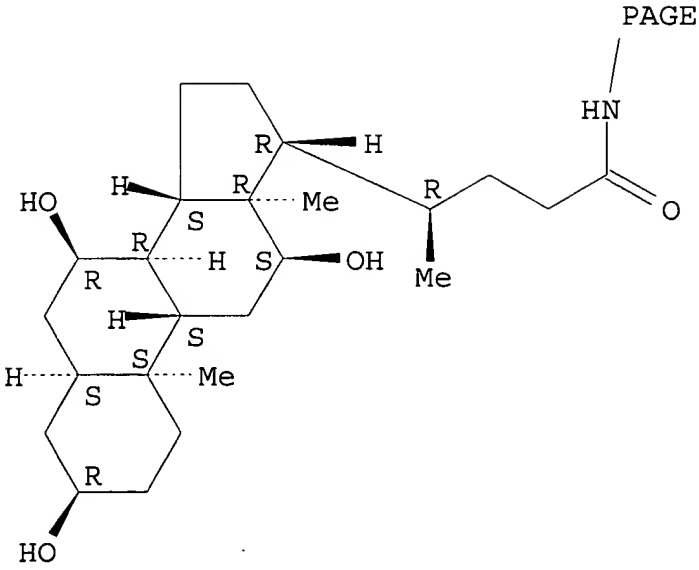
PAGE 1-B



PAGE 1-C



PAGE 2-A



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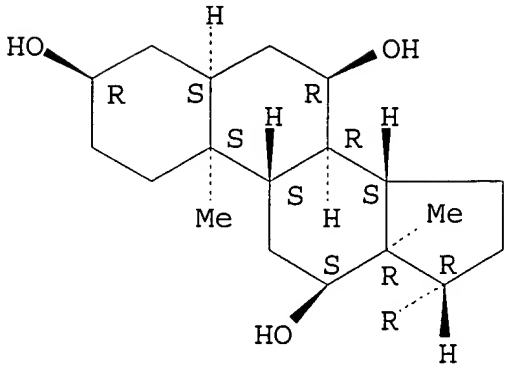
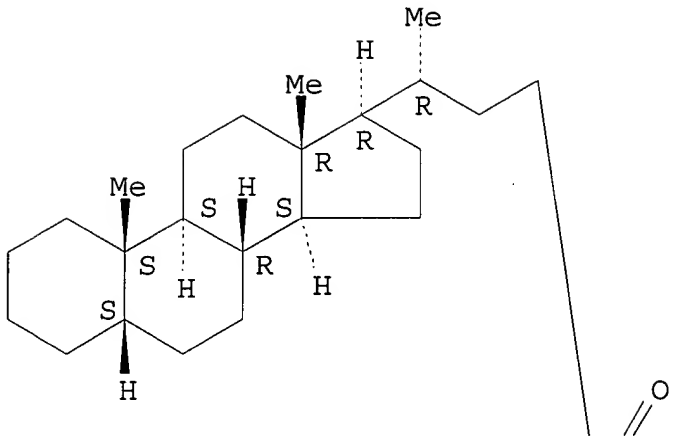


● 4 HCl

RN 351531-44-7 ZCA
CN Cholan-24-amide, N,N',N'',N'''-[7,12,22,27-tetraazapentacyclo[26.2.2.23,6.213,16.218,21]octatriaconta-3,5,13,15,18,20,28,30,31,33,35,37-dodecaene-7,12,22,27-tetrayltetrakis[(1S)-1-(4-aminobutyl)-2-oxo-2,1-ethanediyl]]tetrakis-, tetrahydrochloride (9CI) (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A



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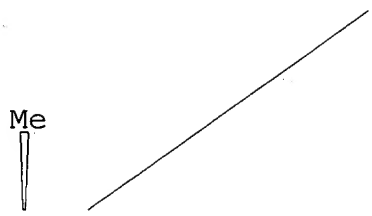
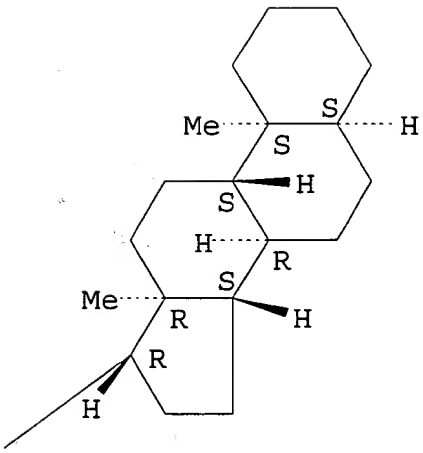
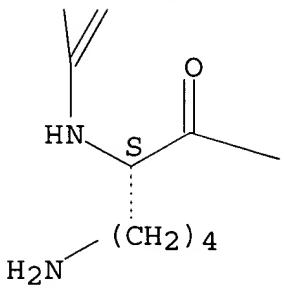
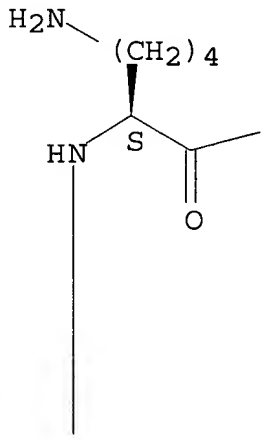


PAGE 1-C



PAGE 2-A





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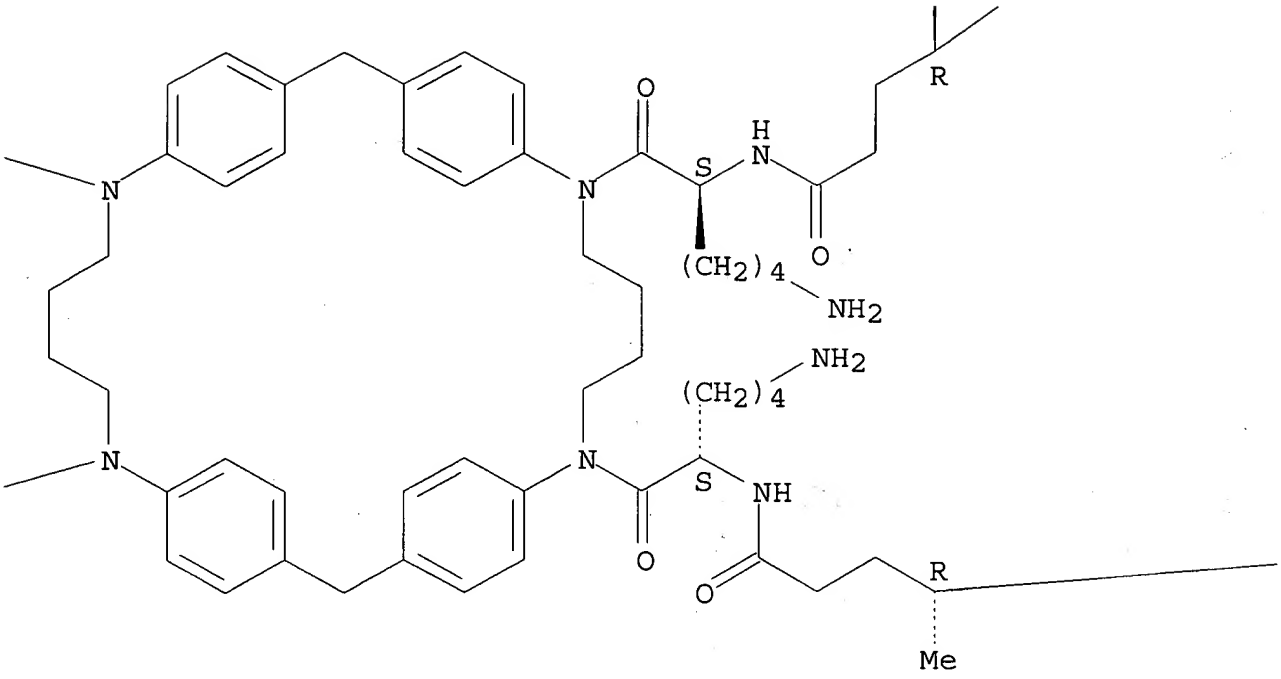

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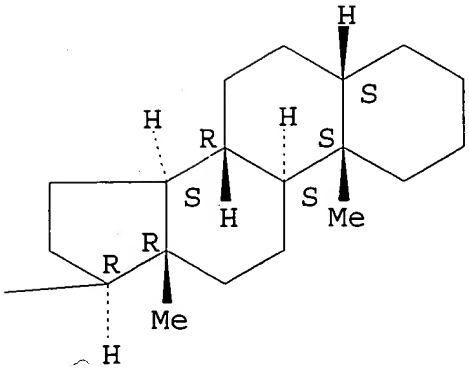
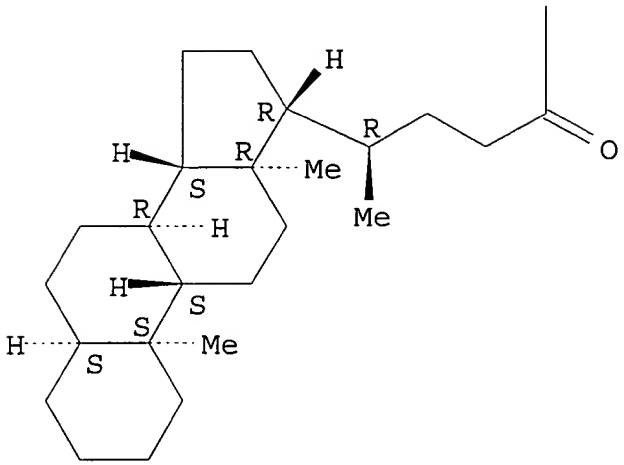


PAGE 3-A



● 4 HCl

IT **156842-46-5 351531-44-7**
(modulation of photo-signal based on mol. recognition by steroid cyclophane in liq. assembly)

L13 ANSWER 5 OF 27 ZCA COPYRIGHT 2003 ACS
135:137636 Dynamic cavity array of steroid cyclophanes at membrane surface. Ariga, K.; Terasaka, Y.; Tsuji, H.; Sakai, D.; Kikuchi, J. (Nara Institute of Science and Technology (NAIST), Graduate School of Materials Science, Takayama, 630-0101, Japan). Studies in Surface Science and Catalysis, 132(Proceedings of the International Conference on Colloid and Surface Science, 2000), 443-446 (English) 2001. CODEN: SSCTDM. ISSN: 0167-2991. Publisher: Elsevier Science B.V..

AB The authors dynamically controlled the cavity structures of steroid cyclophanes placed at the air-water interface and demonstrated repeatable piezoluminescence based on mol. recognition. The repeated compression and expansion of the monolayer of a colic-type steroid cyclophane induced a periodic change in the fluorescence intensity increase upon binding of a fluorescent guest. We also investigated binding of the fluorescent guest in aq. mixts. of the steroid cyclophane and an artificial lipid. Emission wavelength of the fluorescent guest in the mixts. was significantly altered by controlling the mixing ratios.

IT **351531-44-7**
(piezoluminescence based on mol. recognition by dynamic cavity array of steroidal cyclophanes at the air-water interface and in lipid mixts.)

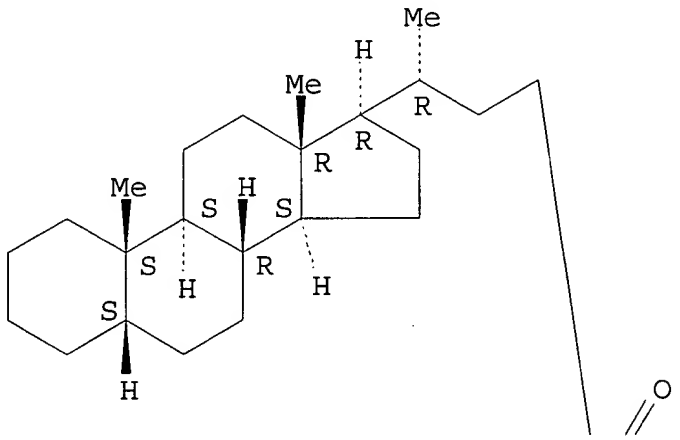
RN 351531-44-7 ZCA

CN Cholan-24-amide, N,N',N'',N'''-[7,12,22,27-tetraazapentacyclo[26.2.2.23,6.213,16.218,21]octatriaconta-

3,5,13,15,18,20,28,30,31,33,35,37-dodecaene-7,12,22,27-tetrayltetrakis[(1S)-1-(4-aminobutyl)-2-oxo-2,1-ethanediyl]]tetrakis-, tetrahydrochloride (9CI) (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A



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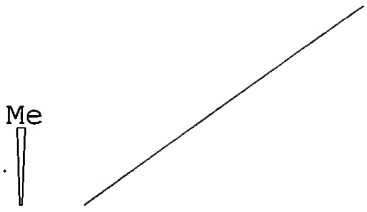

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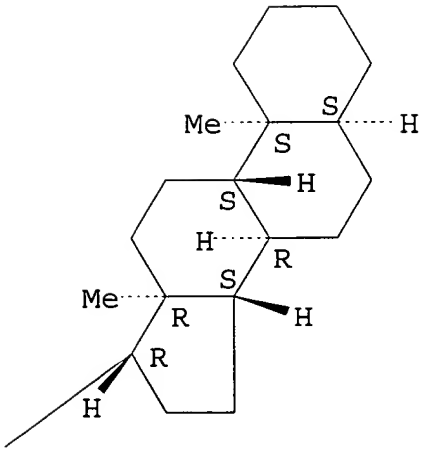

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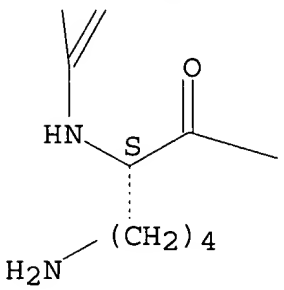

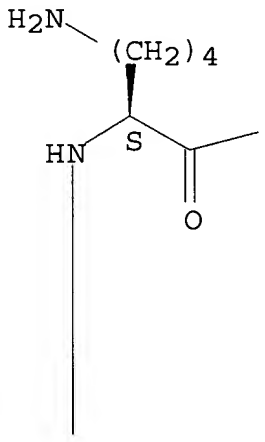

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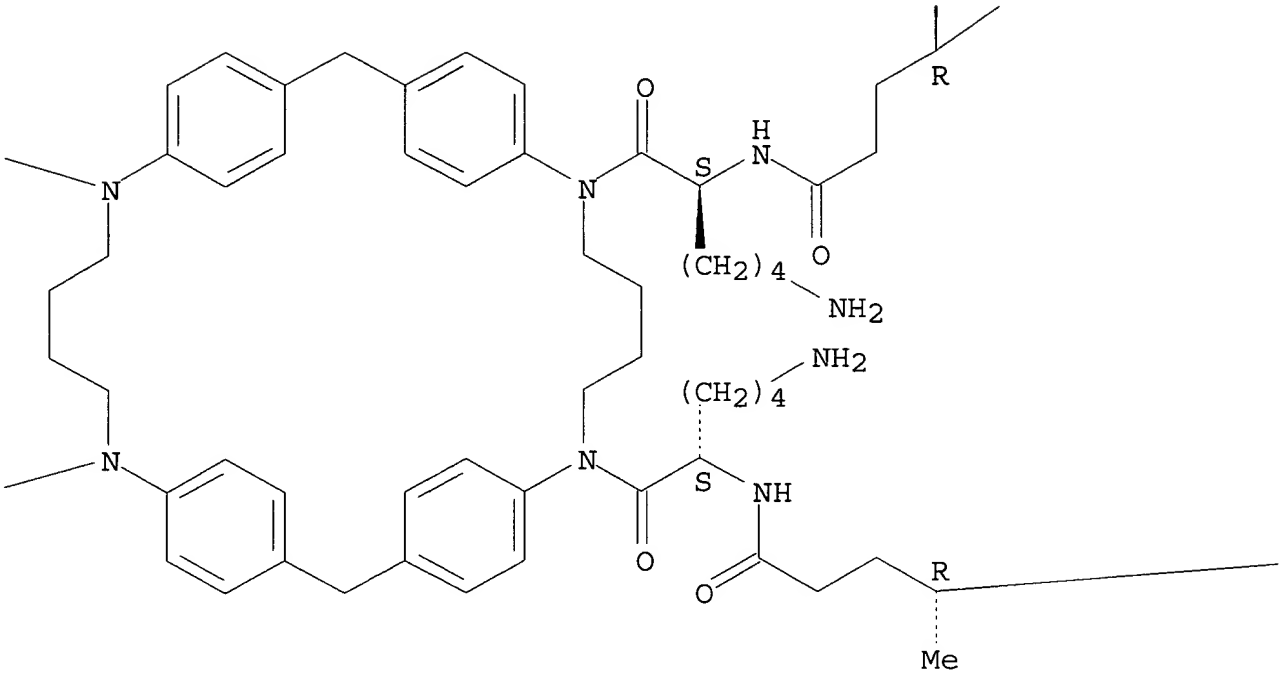
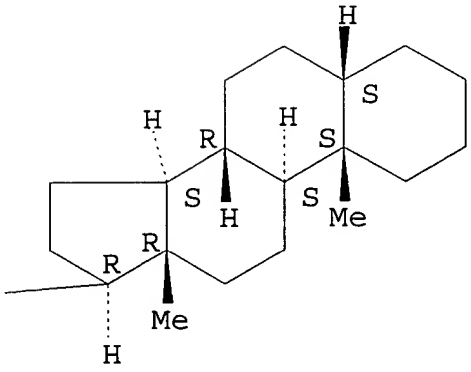


PAGE 2-C



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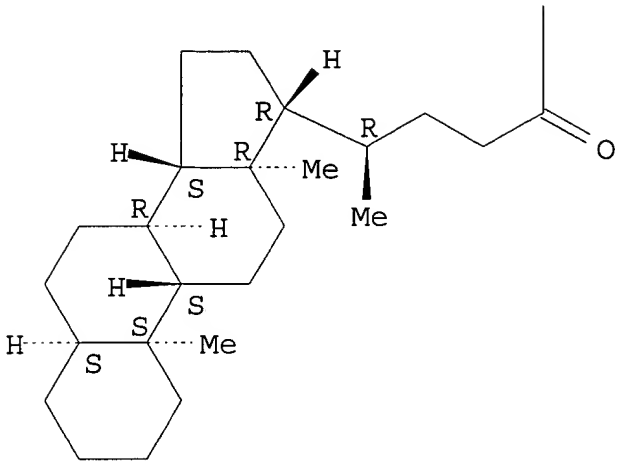


● 4 HCl

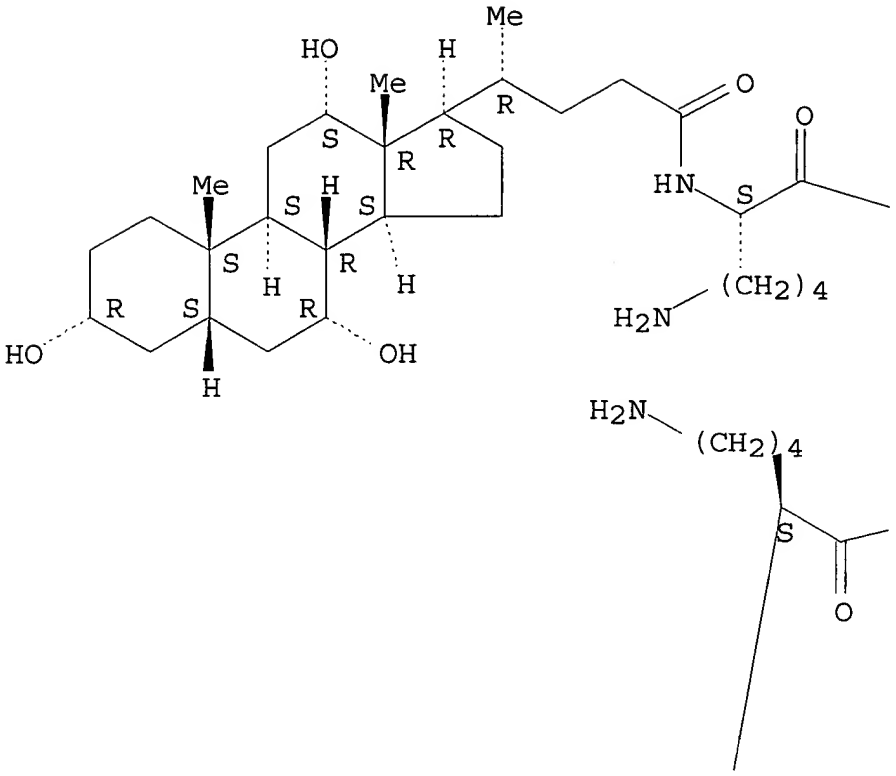
IT **156842-46-5**
(piezoluminescence based on mol. recognition by dynamic cavity array of steroidal cyclophanes at the air-water interface and in lipid mixts.)

RN 156842-46-5 ZCA

CN Cholan-24-amide, N,N',N'',N'''-[7,12,22,27-tetraazapentacyclo[26.2.2.23,6.213,16.218,21]octatriaconta-3,5,13,15,18,20,28,30,31,33,35,37-dodecaene-7,12,22,27-tetrayltetrakis[1-(4-aminobutyl)-2-oxo-2,1-ethanediyl]]tetrakis[3,7,12-trihydroxy-, tetrahydrochloride, stereoisomer (9CI) (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A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Me
O
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R
R
O
HN
S
Me
S
H
S
S
R
H
H
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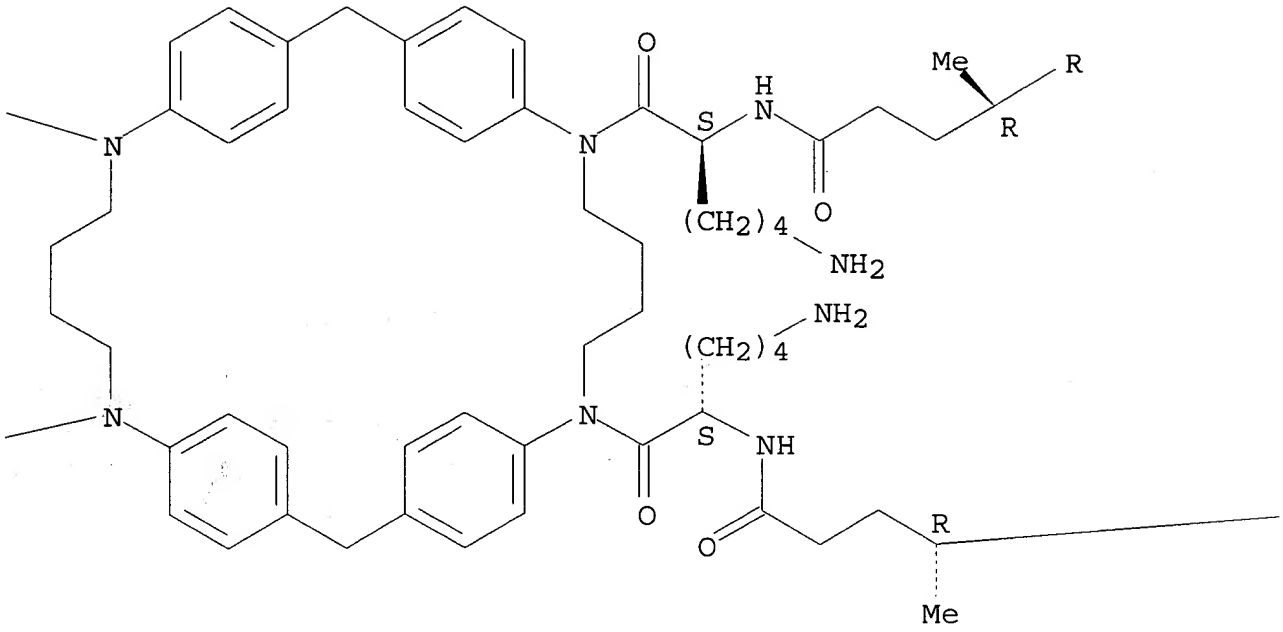
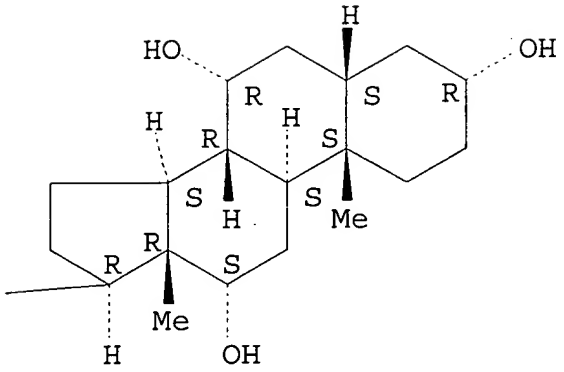
H2N
R
S
H
R
HO
OH
H
H2N
(CH2)4
S
O

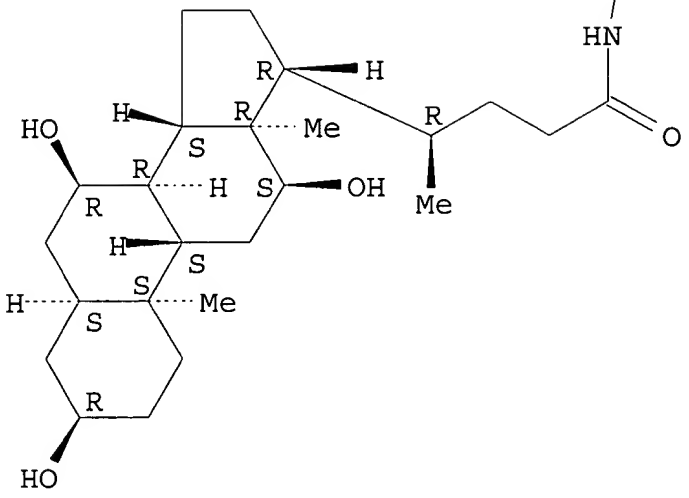
PAGE 1-B



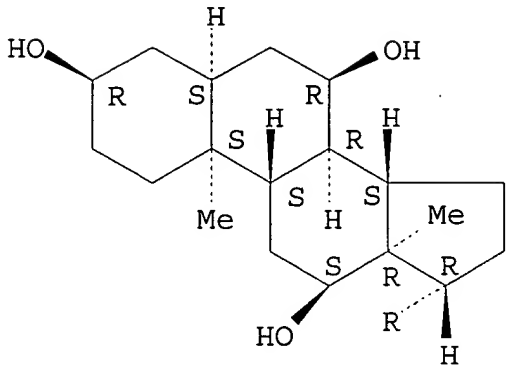
PAGE 1-C



PAGE 2-A



PAGE 3-A



● 4 HCl

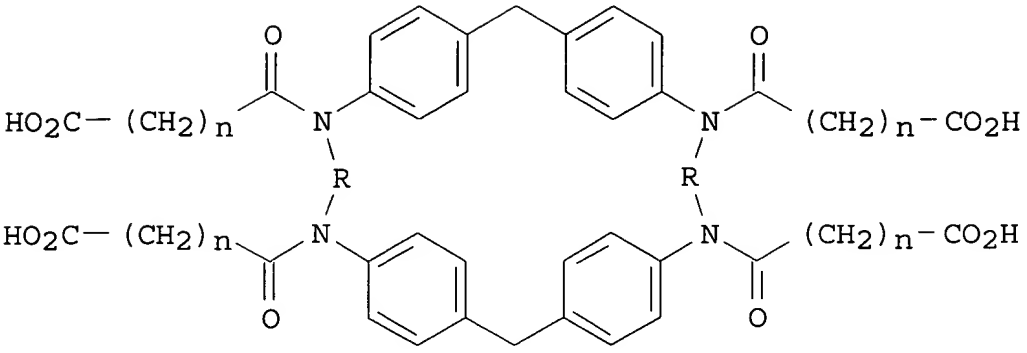
IT **351531-44-7**
(piezoluminescence based on mol. recognition by dynamic cavity array of steroidal cyclophanes at the air-water interface and in lipid mixts.)

IT **156842-46-5**
(piezoluminescence based on mol. recognition by dynamic cavity array of steroidal cyclophanes at the air-water interface and in lipid mixts.)

L13 ANSWER 6 OF 27 ZCA COPYRIGHT 2003 ACS

134:193457 Use of chemical chelators as reversal agents for drug-induced neuromuscular block. Bom, Antonius Helena Adolf; Muir, Alan William; Rees, David (Akzo Nobel N.V., Neth.). PCT Int. Appl. WO 2001012202 A2 20010222, 30 pp. DESIGNATED STATES: W: AL, AU, BA, BB, BG, BR, CA, CN, CU, CZ, EE, GE, HR, HU, ID, IL, IN, IS, JP, KP, KR, LC, LK, LR, LT, LV, MG, MK, MN, MX, NO, NZ, PL, RO, RU, SG, SI, SK, SL, TR, TT, UA, US, UZ, VN, YU, ZA, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM; RW: AT, BE, BF, BJ, CF, CG, CH, CI, CM, CY, DE, DK, ES, FI, FR, GA, GB, GR, IE, IT, LU, MC, ML, MR, NE, NL, PT, SE, SN, TD, TG. (English). CODEN: PIXXD2. APPLICATION: WO 2000-EP7694 20000807. PRIORITY: EP 1999-306411 19990813.

GI



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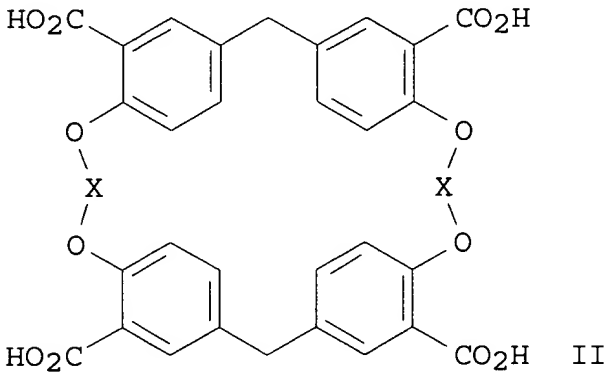


II

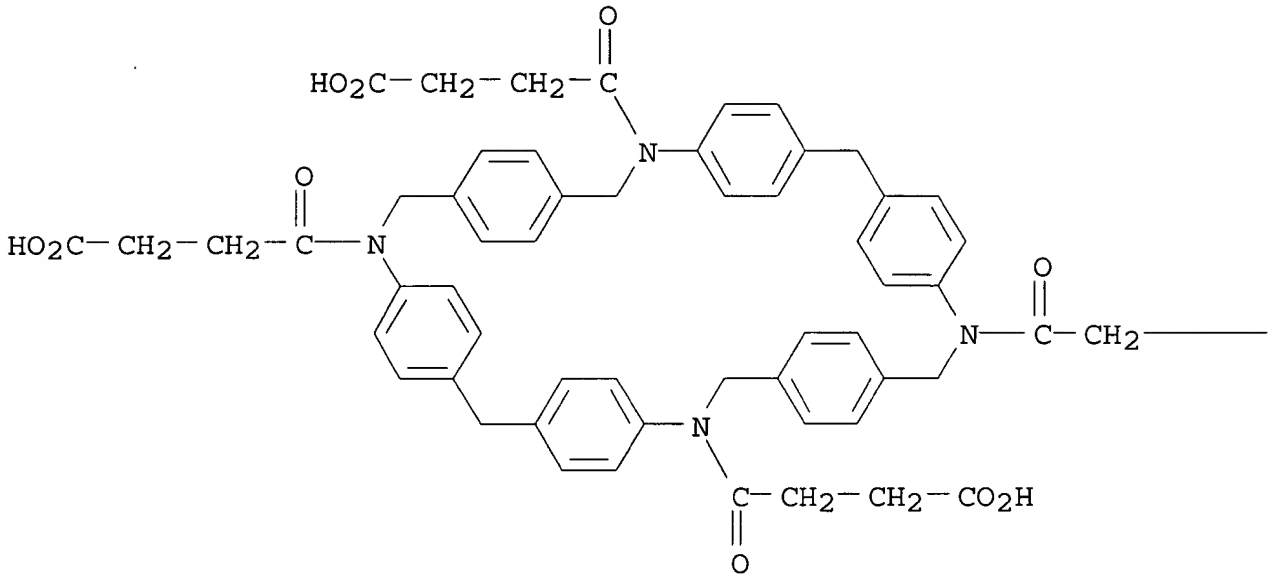
AB Cyclophanes I [R = (CH2)5, 4-CH2C6H4CH2, 1,4-cyclohexanediyldimethylene; n = 1, 2, 3] and II [X = (CH2)5, 4-CH2C6H4CH2, 2,6-naphthalenediyldimethylene] were prepd. Thus, the tetra-Me ester of I [R = (CH2)5, n = 2] was prepd. from 1,7,21,27-tetraaza[7.1.7.1]paracyclophane and 3-(methoxycarbonyl)propionyl chloride and was sapond. to give the tetracarboxylic acid. Both in vivo tests of cyclodextrin derivs. and in vitro tests of I, II, and cyclodextrin derivs. as reversal agents for drug-induced neuromuscular block were described.

IT **327028-12-6P 327028-13-7P**
(chem. chelators as reversal agents for drug-induced neuromuscular block)

RN 327028-12-6 ZCA

CN 7,14,24,31-Tetraazaheptacyclo[30.2.2.23,6.29,12.215,18.220,23.226,29]hexatetraconta-3,5,9,11,15,17,20,22,26,28,32,34,35,37,39,41,43,45-octadecaene-7,14,24,31-tetrabutanoic acid, .gamma.,.gamma.',.gamma.'',.gamma.'''-tetraoxo- (9CI) (CA INDEX NAME)

PAGE 1-A

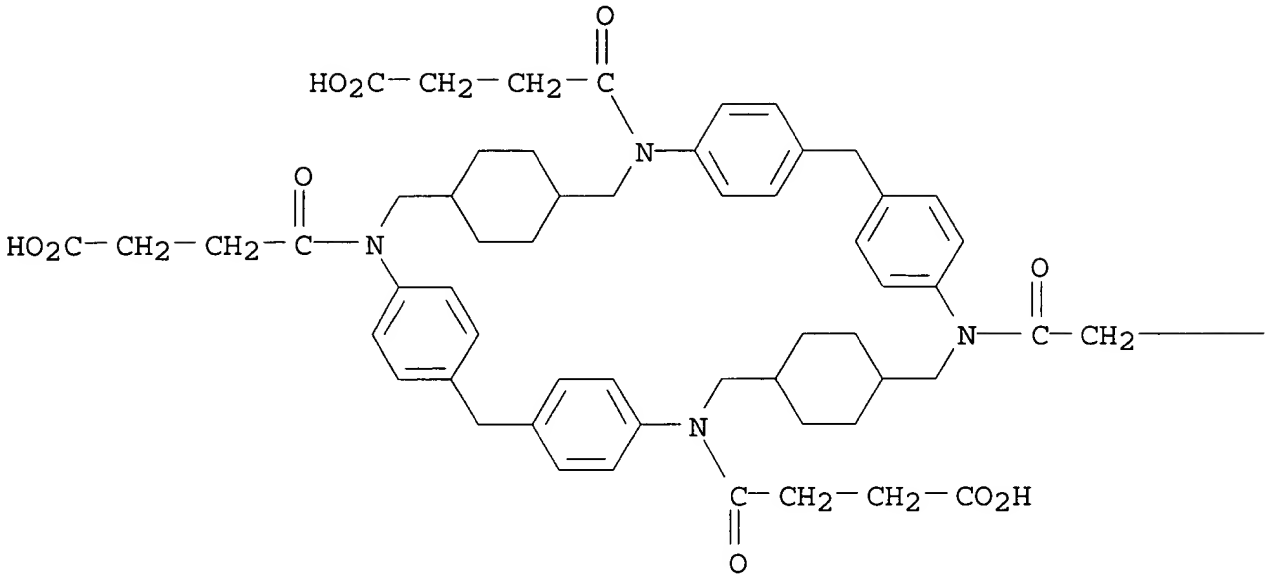


PAGE 1-B

— CH_2— CO_2H

RN 327028-13-7 ZCA
CN 7,14,24,31-Tetraazaheptacyclo[30.2.2.23,6.29,12.215,18.220,23.226,29]hexatetraconta-3,5,15,17,20,22,32,34,35,39,41,45-dodecaene-7,14,24,31-tetrabutanoic acid, .gamma.,.gamma.',.gamma.'',.gamma.'''-tetraoxo- (9CI) (CA INDEX NAME)

PAGE 1-A



PAGE 1-B

— CH_2— CO_2H

IT **327028-12-6P 327028-13-7P**
(chem. chelators as reversal agents for drug-induced neuromuscular block)

L13 ANSWER 7 OF 27 ZCA COPYRIGHT 2003 ACS
133:252600 Piezoluminescence Based on Molecular Recognition by Dynamic Cavity Array of Steroid Cyclophanes at the Air-Water Interface. Ariga, Katsuhiko; Terasaka, Yukiko; Sakai, Daisuke; Tsuji, Hiromitsu; Kikuchi, Jun-ichi (Graduate School of Materials Science, Nara Institute of Science and Technology (NAIST), Ikoma Nara, 630-0101, Japan). Journal of the American Chemical Society,

122(32), 7835-7836 (English) 2000. CODEN: JACSAT. ISSN: 0002-7863. Publisher: American Chemical Society.

AB The authors dynamically controlled the cavity structure of 1,6,20,25-tetraaza[6.1.6.1]paracyclophane connected to four cholanic moieties through a flexible L-lysine spacer and demonstrated repeatable piezoluminescence based on mol. recognition of methylphenylaminonaphthalenesulfonic acid.

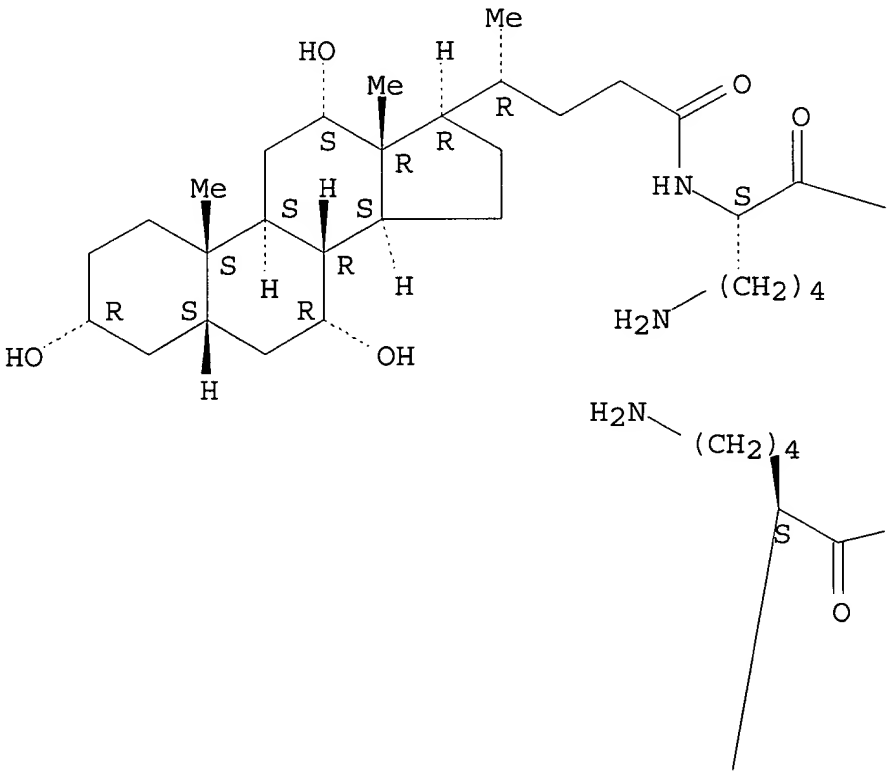
IT **156842-46-5 351531-44-7**
(piezoluminescence based on mol. recognition by dynamic cavity array of steroid cyclophanes at the air-water interface)

RN 156842-46-5 ZCA

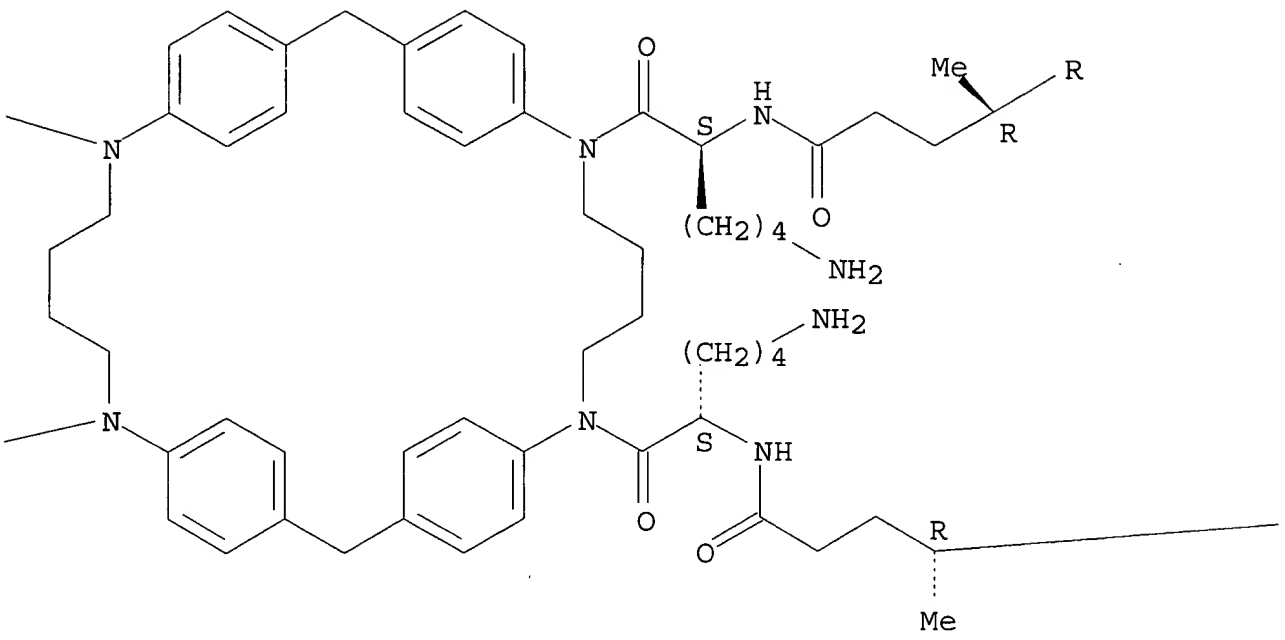
CN Cholan-24-amide, N,N',N'',N'''-[7,12,22,27-tetraazapentacyclo[26.2.2.23,6.213,16.218,21]octatriaconta-3,5,13,15,18,20,28,30,31,33,35,37-dodecaene-7,12,22,27-tetrayltetrakis[1-(4-aminobutyl)-2-oxo-2,1-ethanediyl]]tetrakis[3,7,12-trihydroxy-, tetrahydrochloride, stereoisomer (9CI) (CA INDEX NAME)

Absolute stereochemistry.

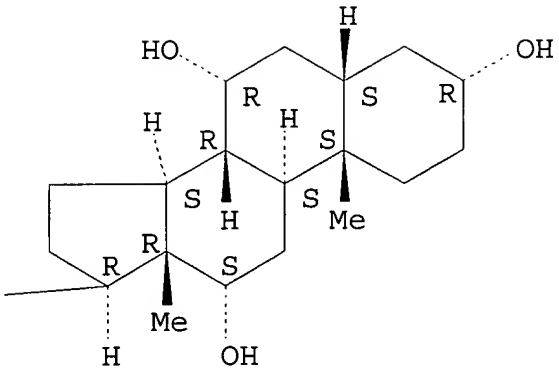
PAGE 1-A



PAGE 1-B



PAGE 1-C



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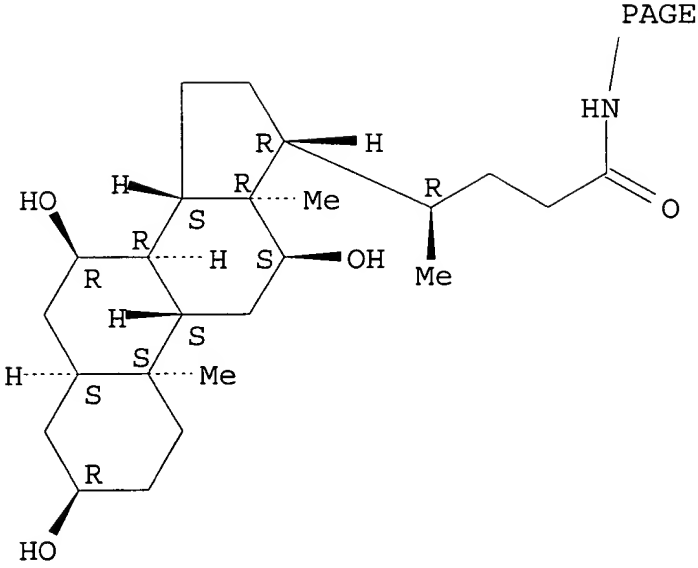
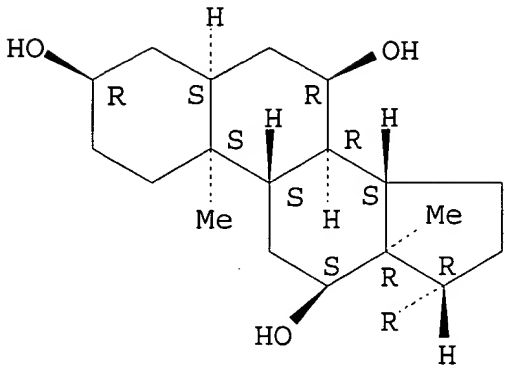


PAGE 3-A

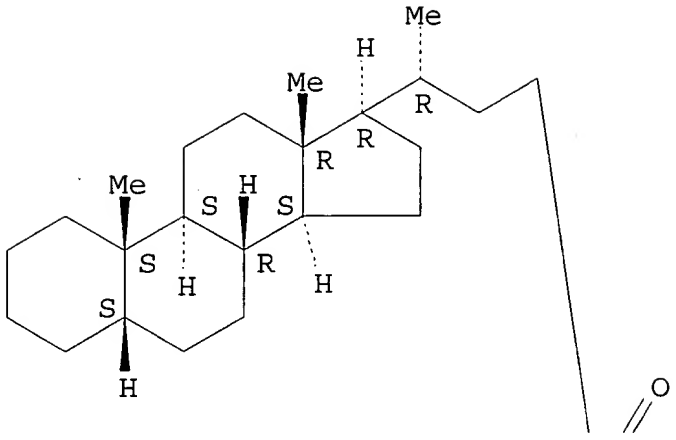


● 4 HCl

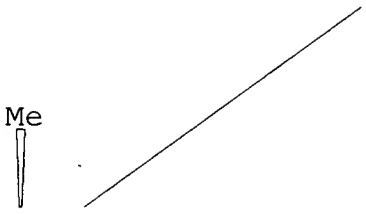
RN 351531-44-7 ZCA
CN Cholan-24-amide, N,N',N'',N'''-[7,12,22,27-tetraazapentacyclo[26.2.2.23,6.213,16.218,21]octatriaconta-3,5,13,15,18,20,28,30,31,33,35,37-dodecaene-7,12,22,27-tetrayltetrakis[(1S)-1-(4-aminobutyl)-2-oxo-2,1-ethanediyl]]tetrakis-, tetrahydrochloride (9CI) (CA INDEX NAME)

Absolute stereochemistry.

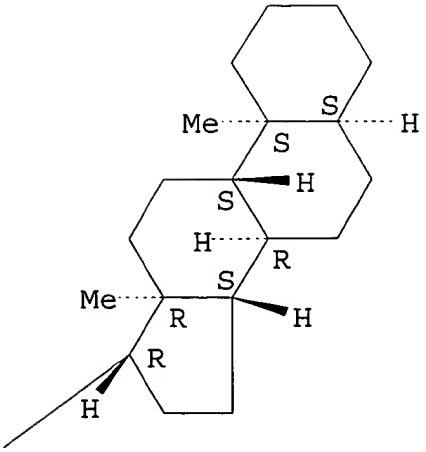
PAGE 1-A



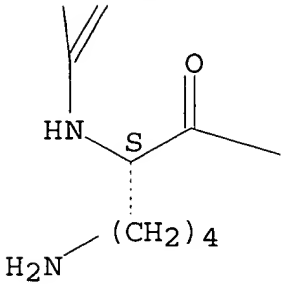
PAGE 1-B

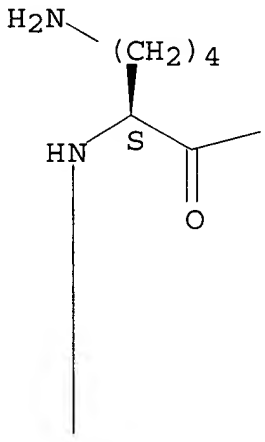


PAGE 1-C

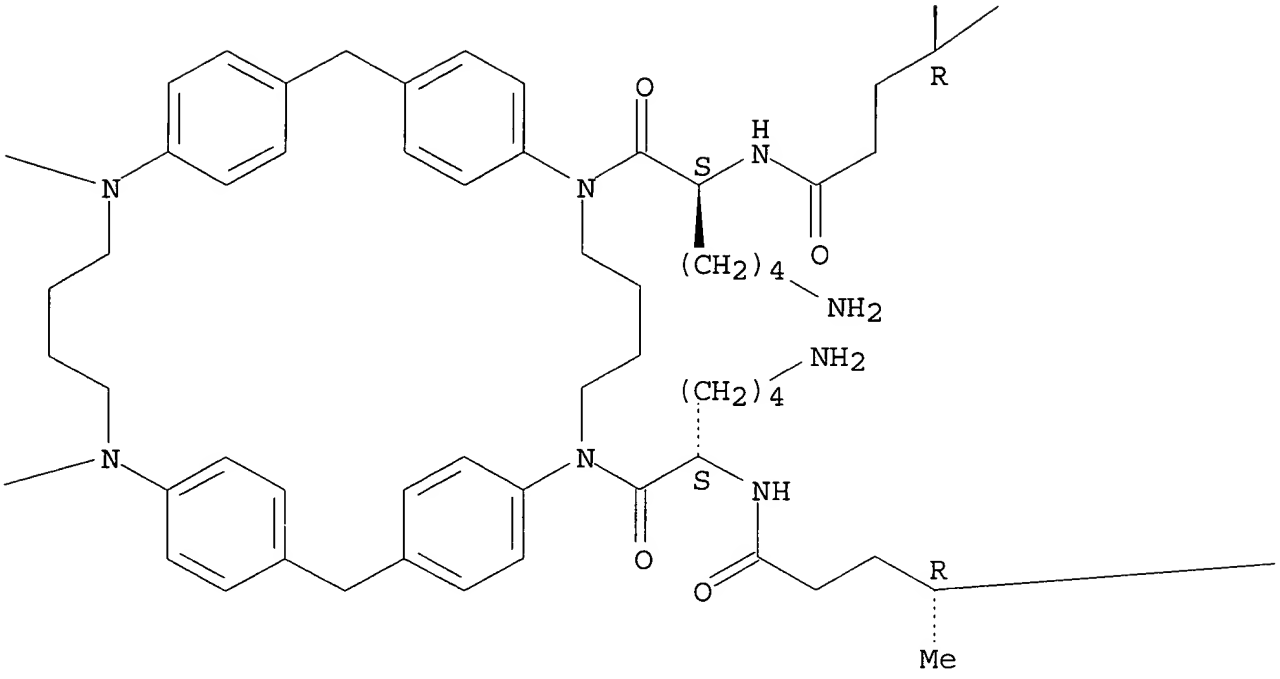


PAGE 2-A





PAGE 2-B



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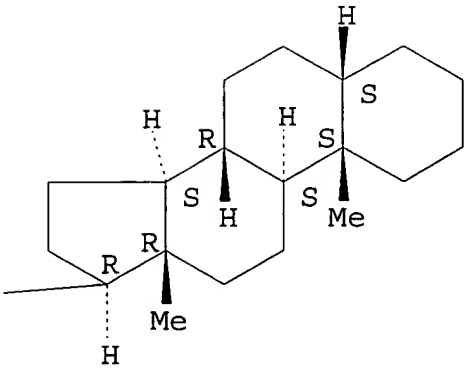

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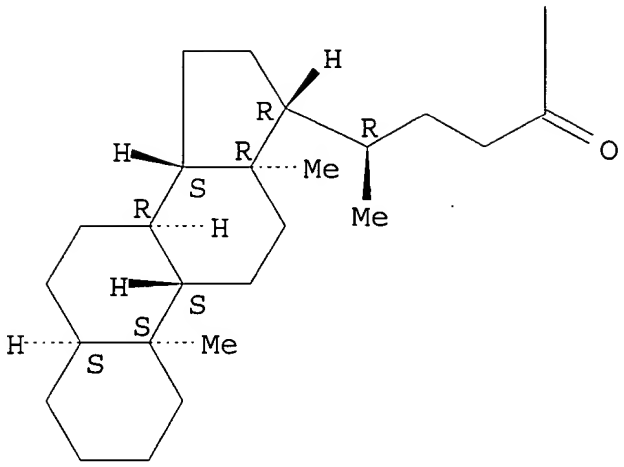


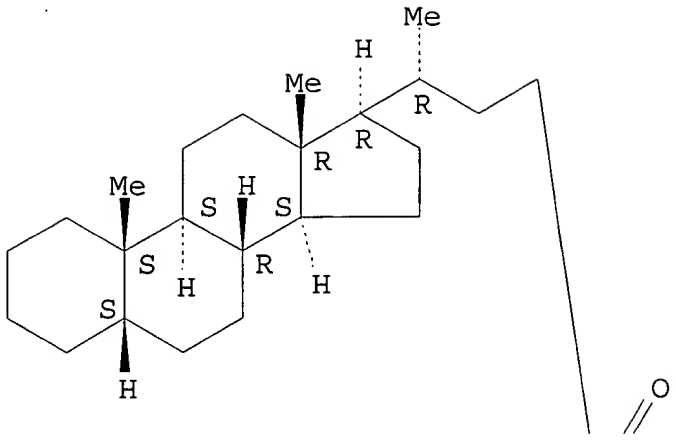
● 4 HCl

IT **156842-46-5 351531-44-7**
(piezoluminescence based on mol. recognition by dynamic cavity array of steroid cyclophanes at the air-water interface)

L13 ANSWER 8 OF 27 ZCA COPYRIGHT 2003 ACS
131:1755 An artificial signal transduction system. Control of lactate dehydrogenase activity performed by an artificial cell-surface receptor. Kikuchi, Jun-ichi; Ariga, Katsuhiko; Miyazaki, Tatsuo; Ikeda, Kouki (Graduate School of Materials Science, Nara Institute of Science and Technology, Nara, 630-0101, Japan). Chemistry Letters (3), 253-254 (English) 1999. CODEN: CMLTAG. ISSN: 0366-7022. Publisher: Chemical Society of Japan.
AB A supramol. bilayer assembly as an artificial signaling system was constituted in combination with a steroid cyclophane as an artificial receptor, an NADH-dependent lactate dehydrogenase as an effector, and a bilayer-forming peptide lipid. Signal transduction from the receptor to the effector was obsd. for the present hybrid system by employing two kinds of signaling species, 1-hydroxy-2-naphthaldehyde as an external signal and a Cu(II) ion as a signal transmitter.
IT **225379-53-3**
(control of lactate dehydrogenase activity performed by an artificial cell-surface receptor)
RN 225379-53-3 ZCA
CN Cholan-24-amide, N,N',N'',N'''-[7,12,22,27-tetraazapentacyclo[26.2.2.23,6.213,16.218,21]octatriaconta-3,5,13,15,18,20,28,30,31,33,35,37-dodecaene-7,12,22,27-tetrayltetrakis[(1S)-1-(4-aminobutyl)-2-oxo-2,1-ethanediyl]]tetrakis-, monohydrochloride (9CI) (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A



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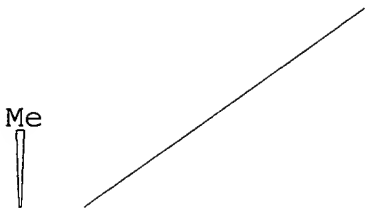

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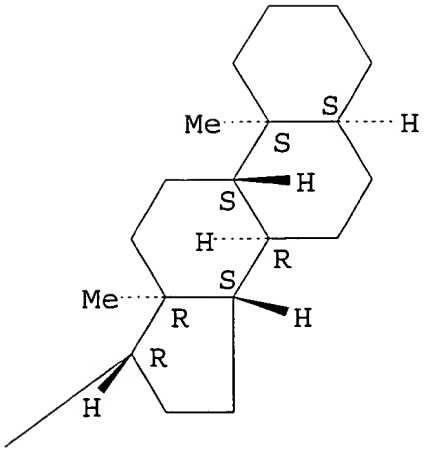

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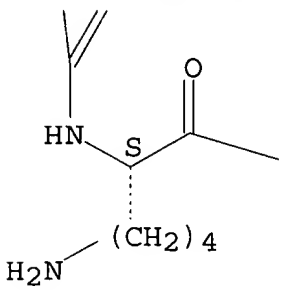

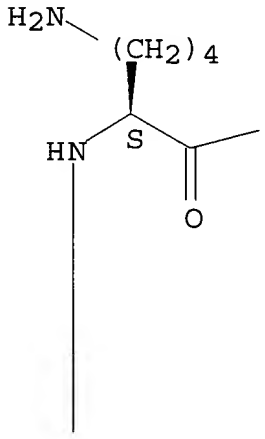

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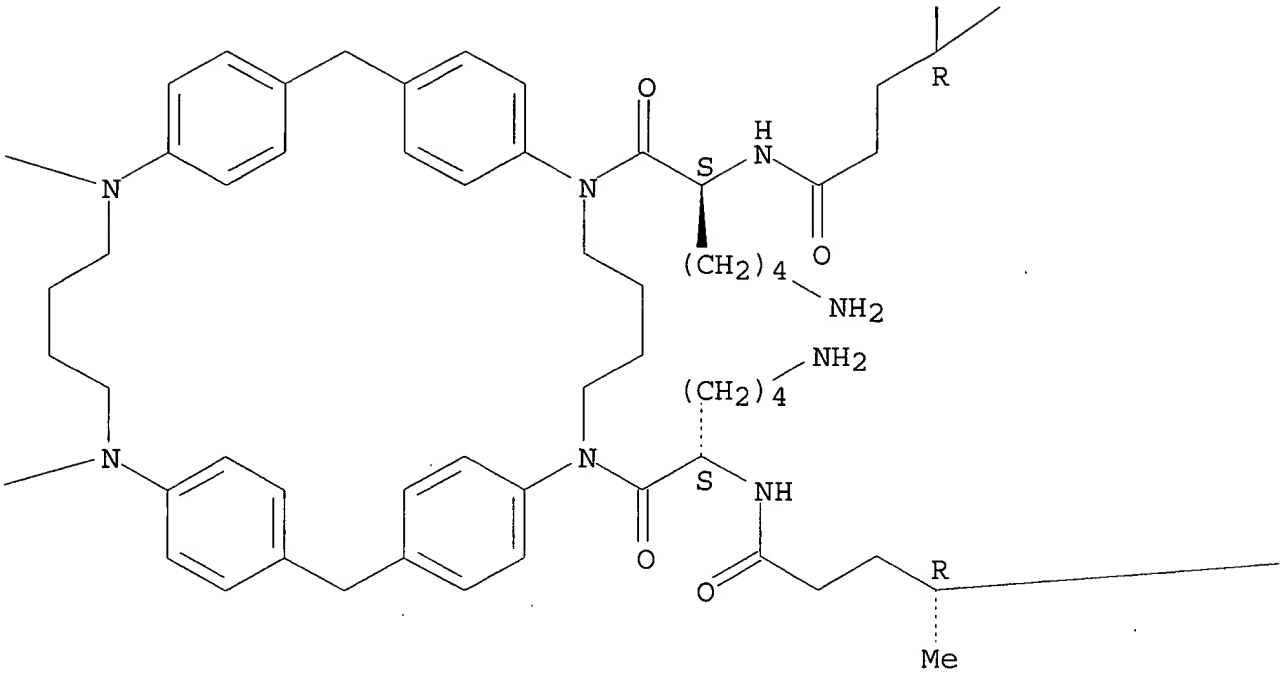

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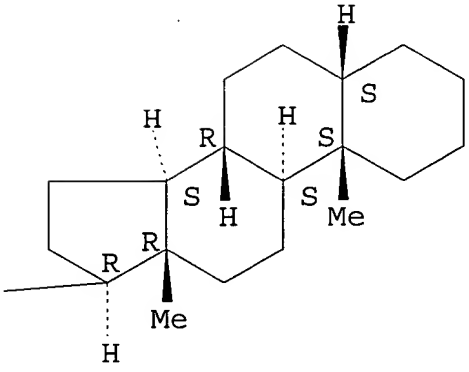

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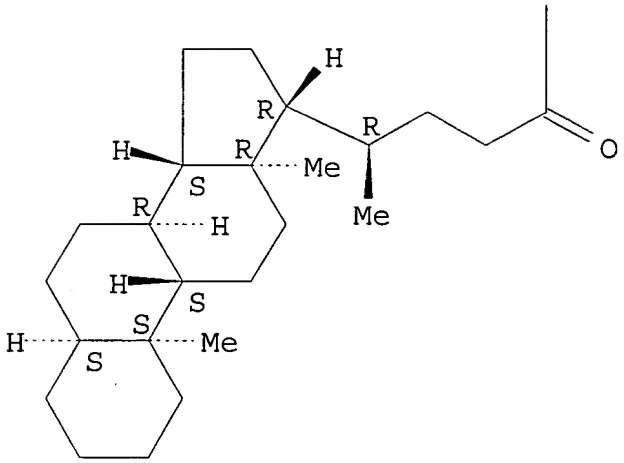


● HCl

IT **225379-53-3**
(control of lactate dehydrogenase activity performed by an artificial cell-surface receptor)

L13 ANSWER 9 OF 27 ZCA COPYRIGHT 2003 ACS
130:278125 Signal transmission by artificial receptors embedded in bilayer membranes. Kikuchi, Jun-Ichi (Institute for Fundamental Research of Organic Chemistry, Kyushu University, Fukuoka, 812-81, Japan). Molecular Recognition and Inclusion, Proceedings of the International Symposium on Molecular Recognition and Inclusion, 9th, Lyon, Sept. 7-12, 1996, Meeting Date 1996, 129-134. Editor(s): Coleman, Annette W. Kluwer: Dordrecht, Neth. (English) 1998. CODEN: 67FSAY.

AB The authors designed steroid cyclophanes as artificial cell-surface receptors. Each steroid cyclophane has three functional components: a 1,6,20,25-tetraaza[6.1.6.1]paracyclophane ring, four bile acid moieties and four L-lysine residues connecting them. They employ hydrophobic arom. guests and metal ions as signaling ligands and signal transmitters, resp., for the steroid cyclphanes.

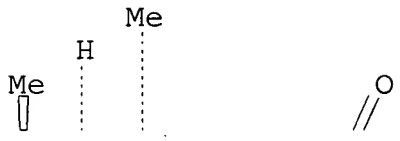
IT **182889-23-2 183072-82-4 220527-51-5 220527-56-0**
(artificial receptor; signal transmission by artificial receptors embedded in bilayer membranes)

RN 182889-23-2 ZCA

CN Cholan-24-amide, N,N',N'',N'''-[7,12,22,27-tetraazapentacyclo[26.2.2.23,6.213,16.218,21]octatriaconta-3,5,13,15,18,20,28,30,31,33,35,37-dodecaene-7,12,22,27-tetrayltetrakis[1-(4-aminobutyl)-2-oxo-2,1-ethanediyl]]tetrakis-, stereoisomer (9CI) (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A



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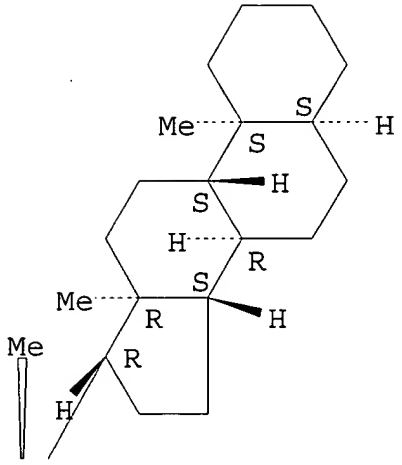

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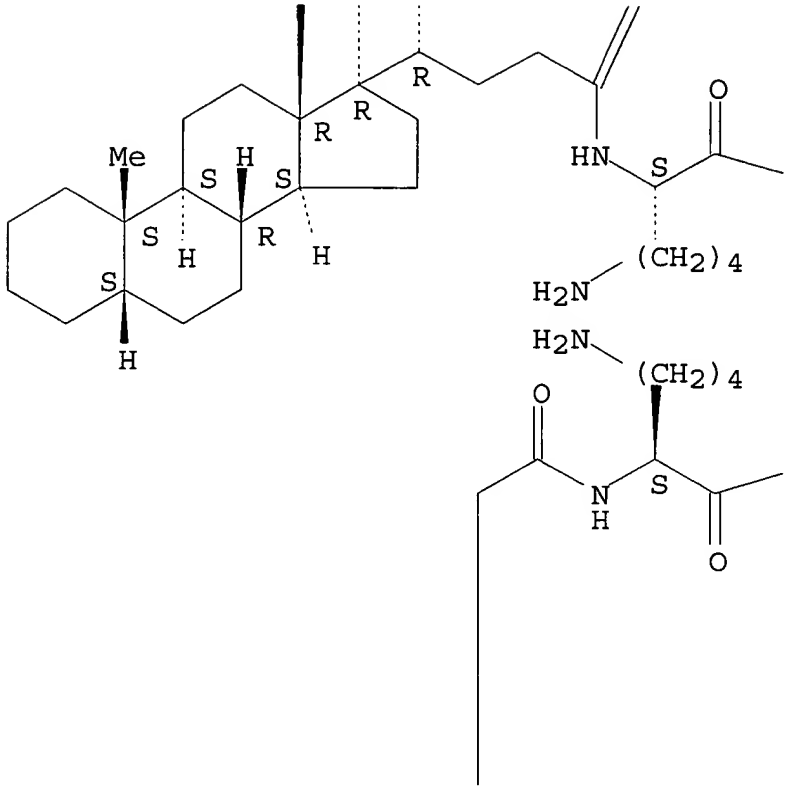

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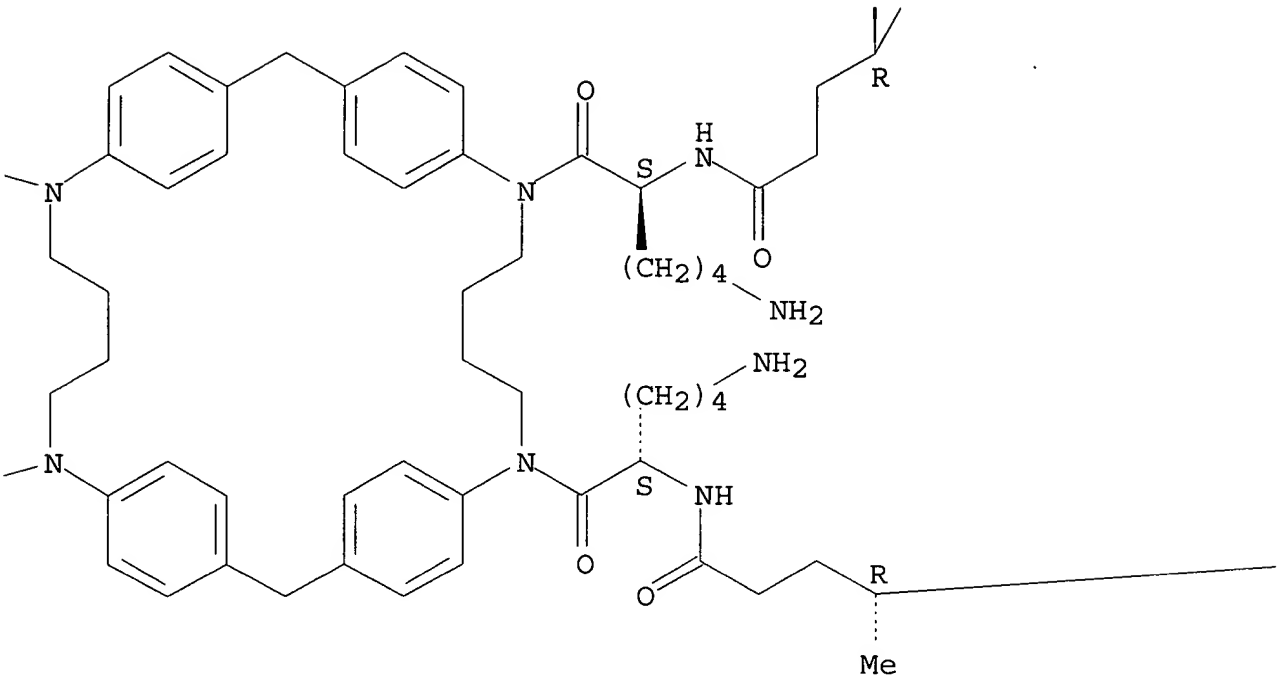

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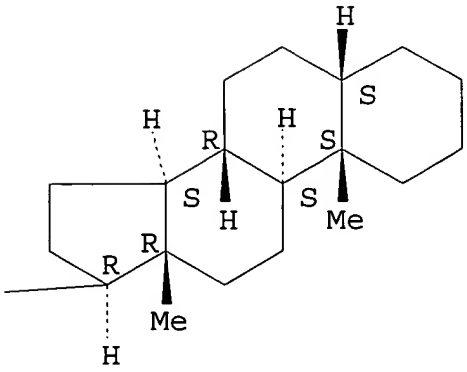

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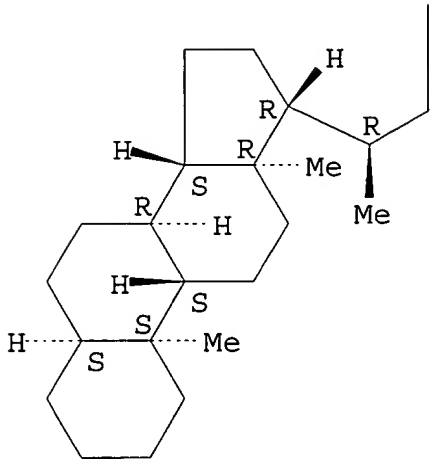

RN 183072-82-4 ZCA
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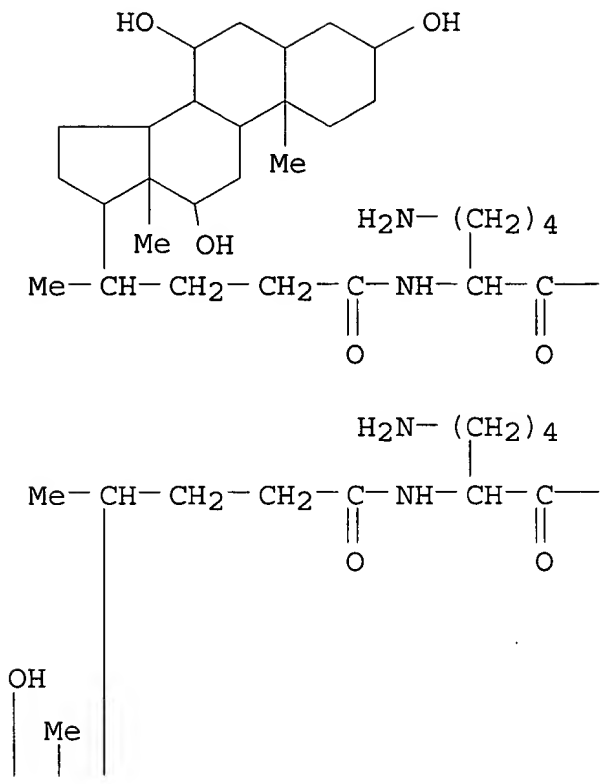
PAGE 1-A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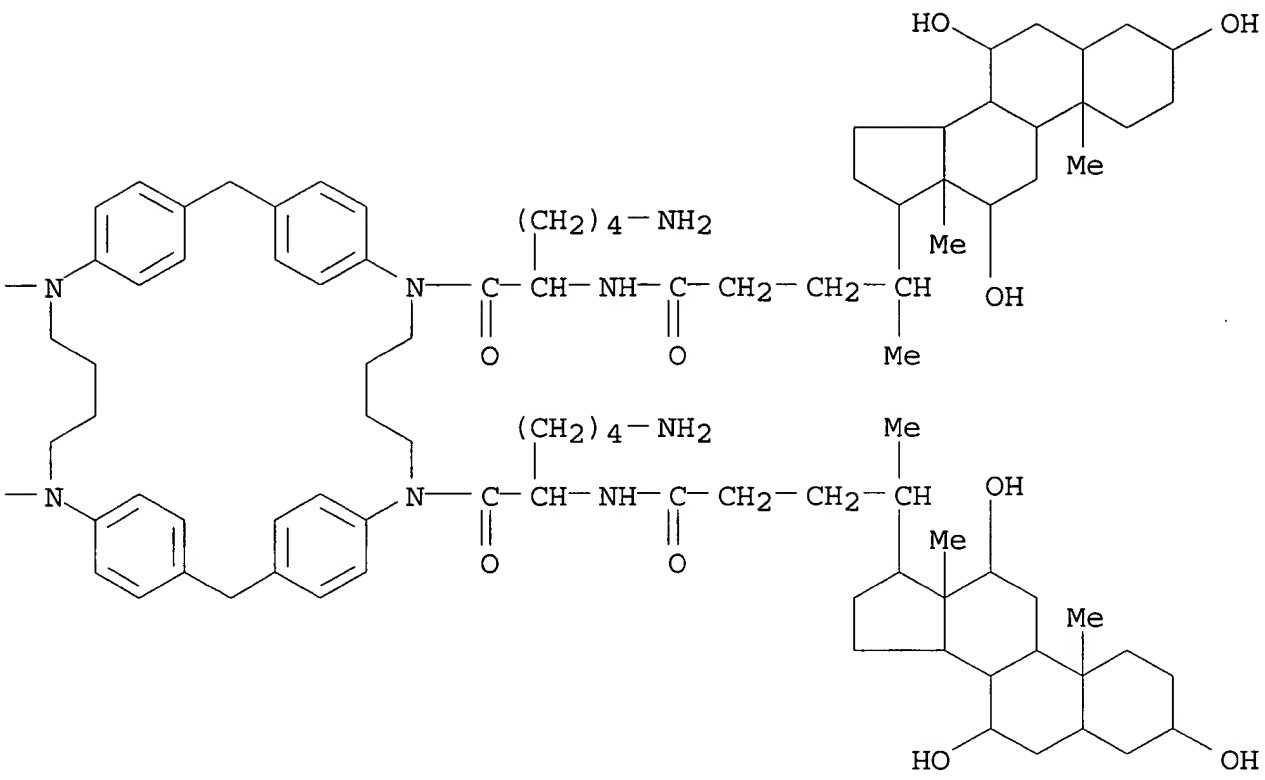
OH
Me
Me
OH
H2N— (CH2)4
Me— CH— CH2— CH2— C— NH— CH— C—
O
O
H2N— (CH2)4
Me— CH— CH2— CH2— C— NH— CH— C—
O
O
OH
Me

PAGE 1-B



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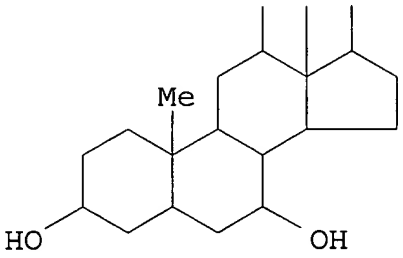

RN 220527-51-5 ZCA
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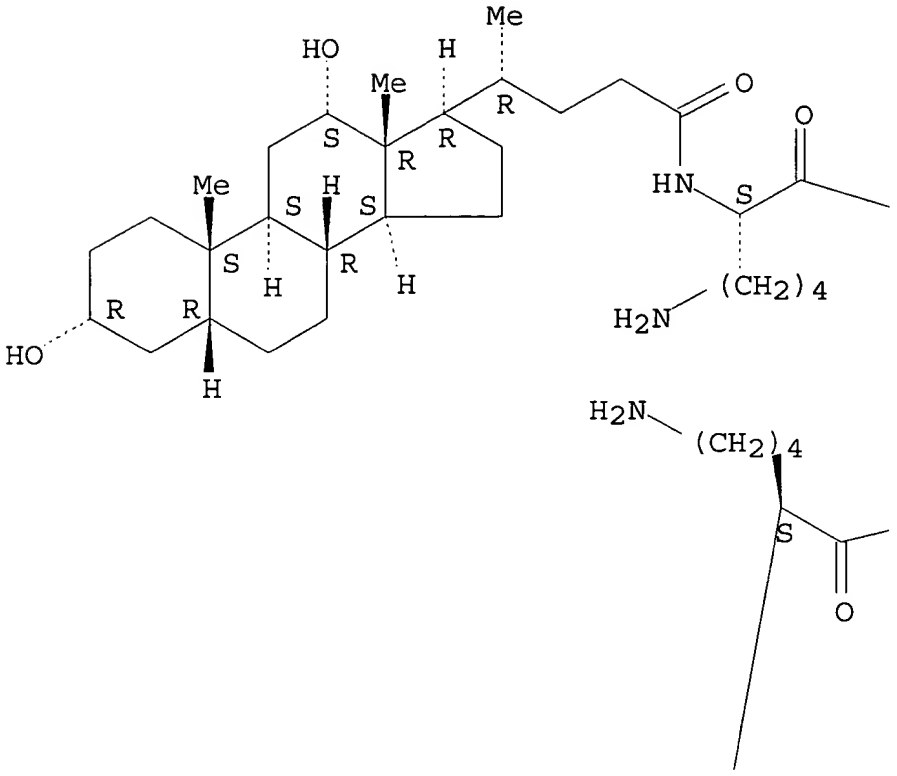
Absolute stereochemistry.

PAGE 1-A



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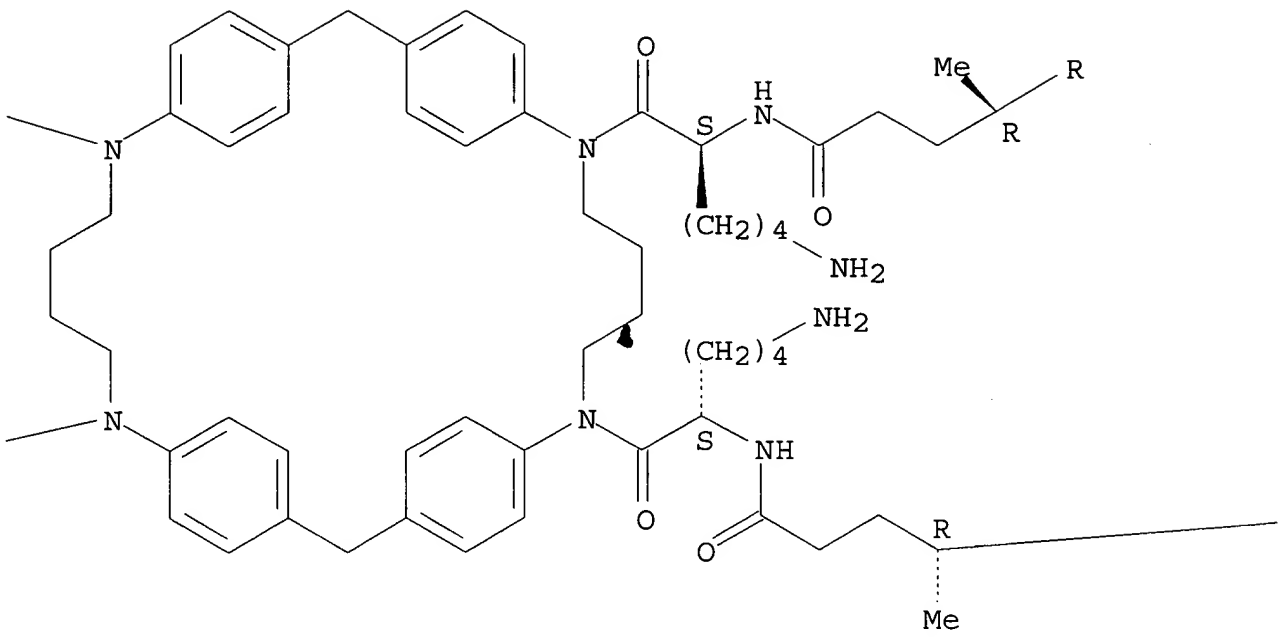

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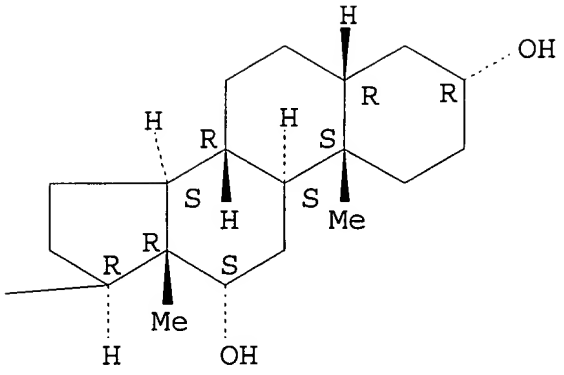

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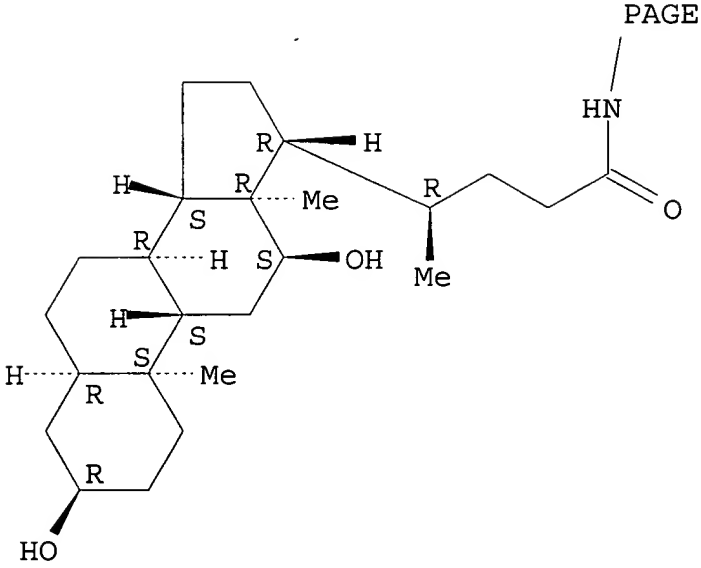

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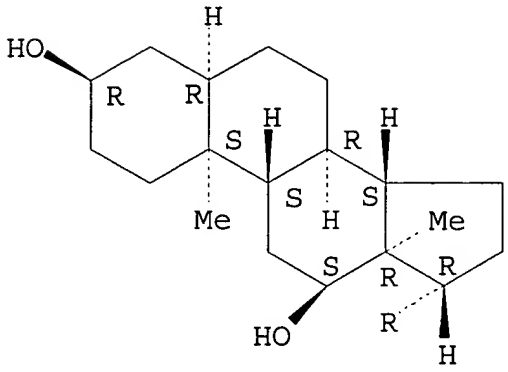

RN 220527-56-0 ZCA
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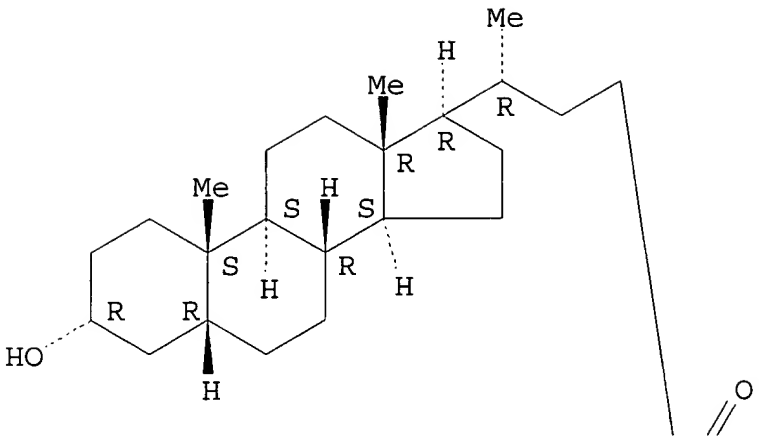
Absolute stereochemistry.

PAGE 1-A



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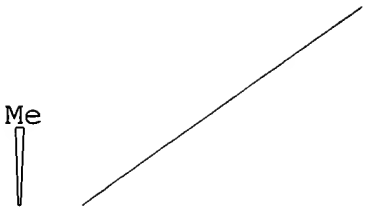

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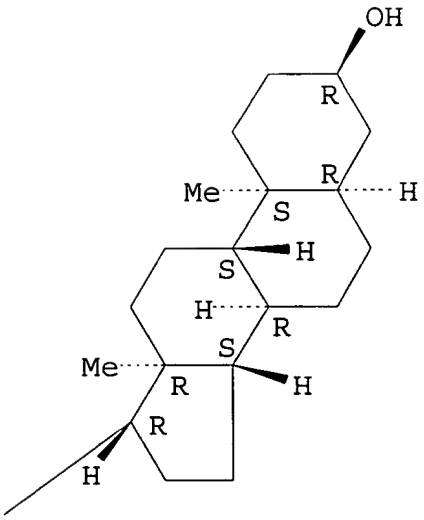
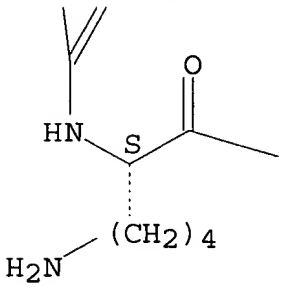
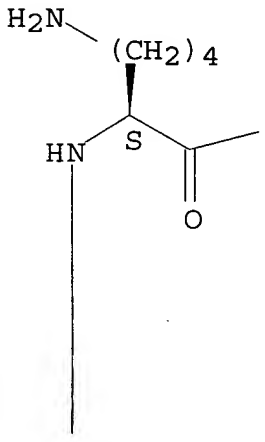


PAGE 2-A





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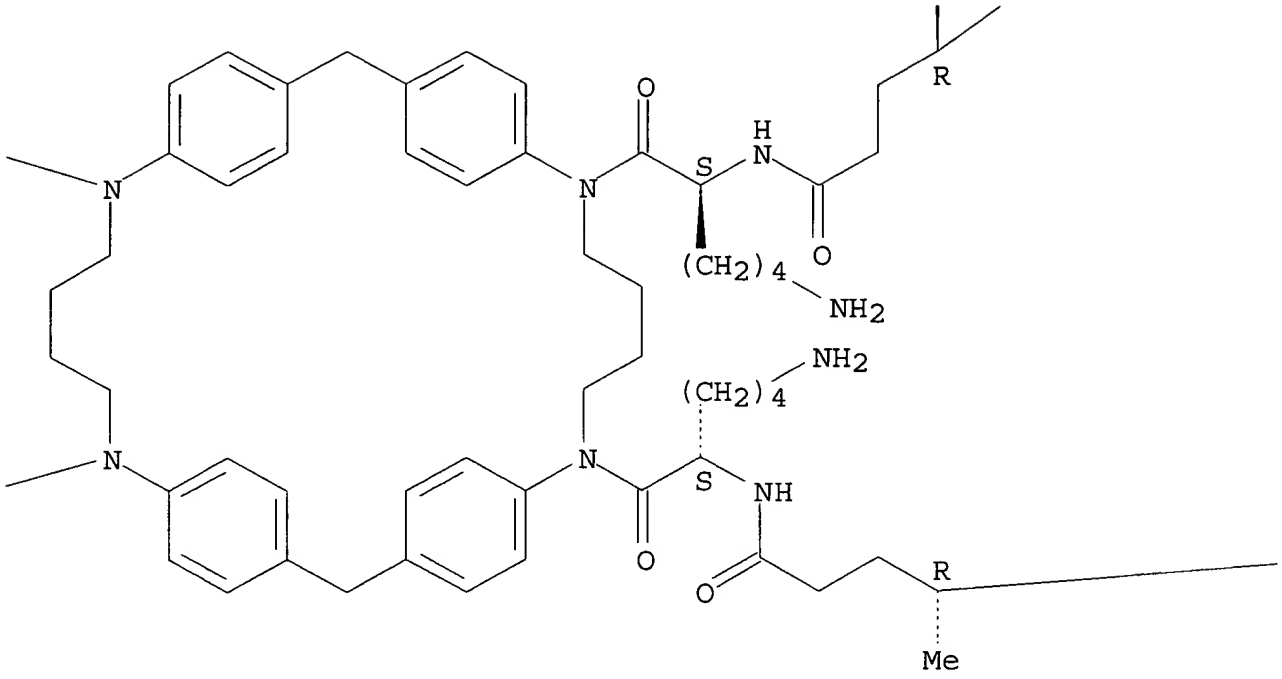

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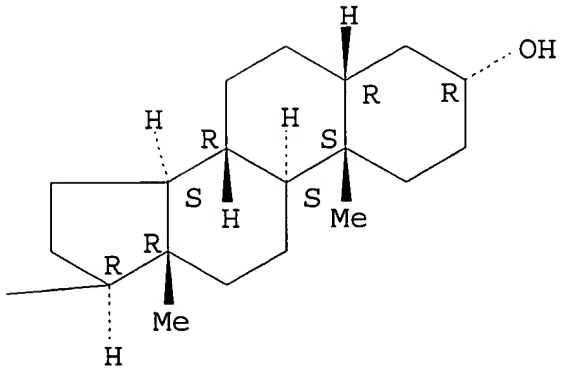

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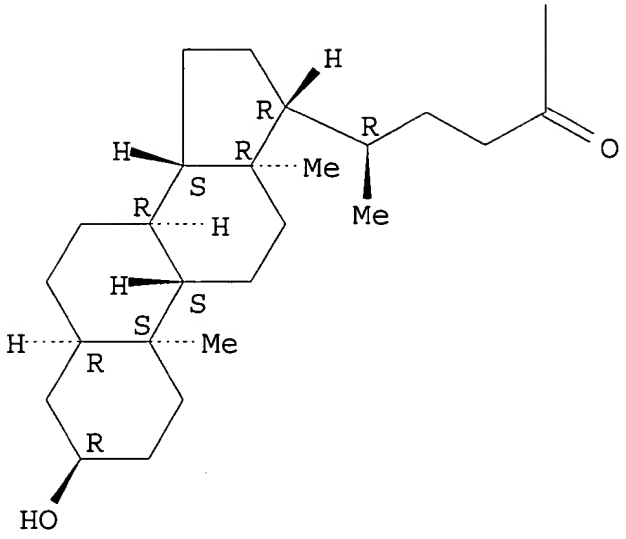


IT **182889-23-2 183072-82-4 220527-51-5**
220527-56-0
(artificial receptor; signal transmission by artificial receptors embedded in bilayer membranes)

L13 ANSWER 10 OF 27 ZCA COPYRIGHT 2003 ACS
130:179092 Steroid cyclophanes as artificial cell-surface receptors. Molecular recognition and its consequence in signal transduction behavior. Kikuchi, Jun-Ichi; Murakami, Yukito (Institute for Fundamental Research in Organic Chemistry, Kyushu University, Fukuoka, 812-8581, Japan). Journal of Inclusion Phenomena and Molecular Recognition in Chemistry, 32(2-3), 209-221 (English) 1998. CODEN: JIMCEN. ISSN: 0923-0750. Publisher: Kluwer Academic Publishers.

AB Steroid cyclophanes, bearing four bile acid moieties covalently placed on a tetraazaparacyclophane skeleton, were designed and synthesized as artificial cell-surface receptors. Guest-binding behavior of the steroid cyclophanes embedded in a bilayer membrane formed with a synthetic peptide lipid was clarified by means of fluorescence and CD spectroscopy. We found that the steroid cyclophane effectively bound arom. guests in both bilayer membranes and aq. soln. In addn., copper(II) ions acted as a guest species for the steroid cyclophane and a competitive inhibitor toward a NADH-dependent lactate dehydrogenase (LDH). On these grounds, we constituted a supramol. assembly as an artificial signaling system in combination with the steroid cyclophane, a cationic peptide lipid, and LDH. As a consequence, the steroid cyclophane acted as an effective artificial cell-surface receptor being capable of transmitting an external signal to the enzyme in collaboration with copper(II) ions as a signal transmitter.

IT **156881-79-7P 182889-23-2P 183072-82-4P**
220527-51-5P 220527-56-0P

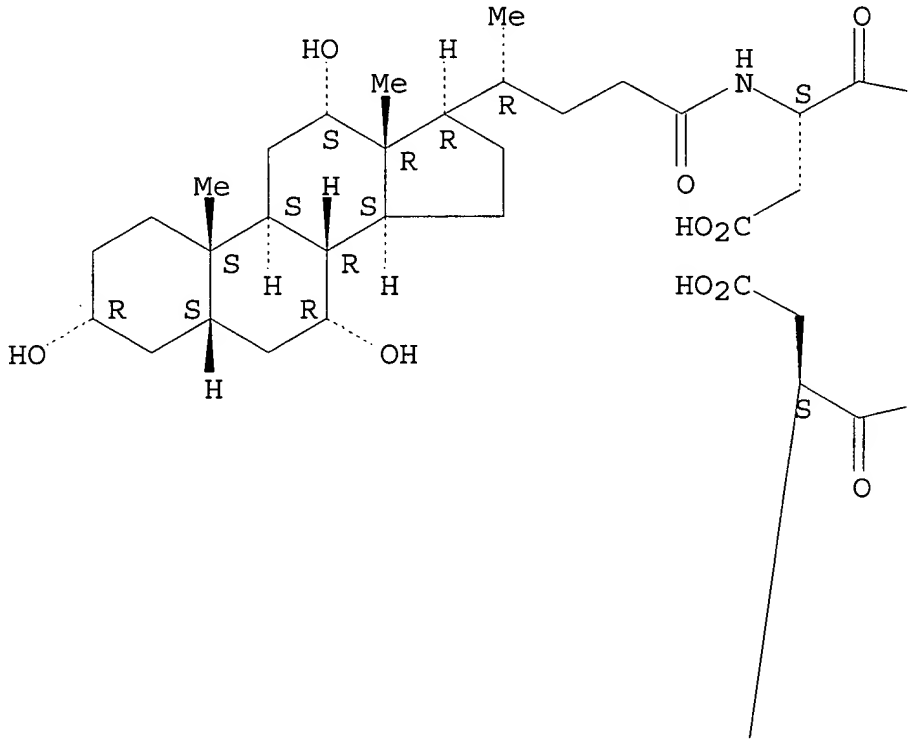
(prepn. and characterization of steroid cyclophanes as artificial cell-surface receptors)

RN 156881-79-7 ZCA

CN 7,12,22,27-Tetraazapentacyclo[26.2.2.23,6.213,16.218,21]octatriaconta-3,5,13,15,18,20,28,30,31,33,35,37-dodecaene-7,12,22,27-tetrabutanoic acid, .gamma.,.gamma.',.gamma.'',.gamma.'''-tetraoxo-.beta.,.beta.',.beta.'',.beta.'''-tetrakis[[(3.alpha.,5.beta.,7.alpha.,12.alpha.)-3,7,12-trihydroxy-24-oxocholan-24-yl]amino]-, (.beta.S,.beta.'S,.beta.''S,.beta.'''S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A



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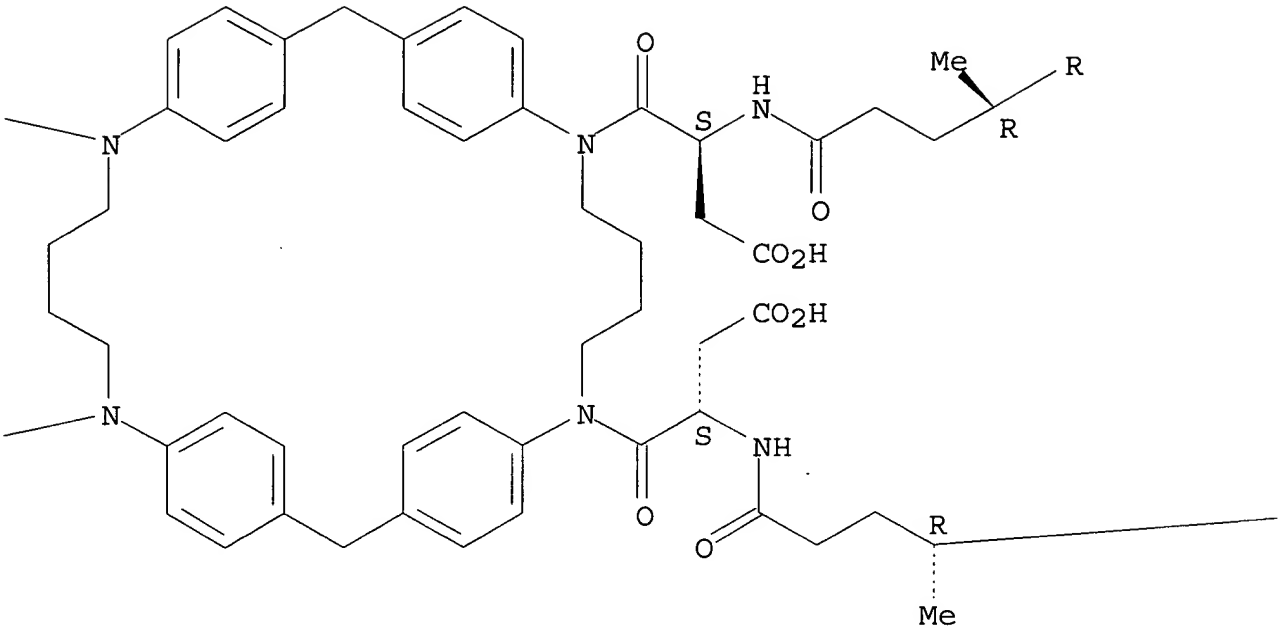

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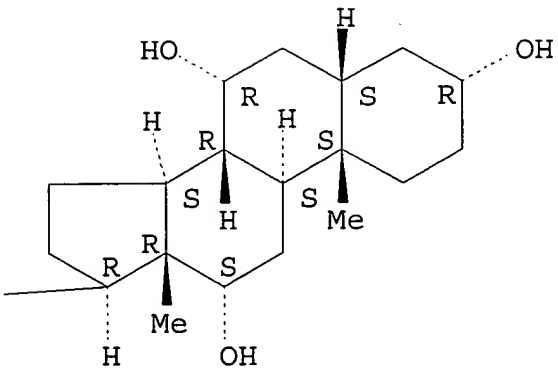

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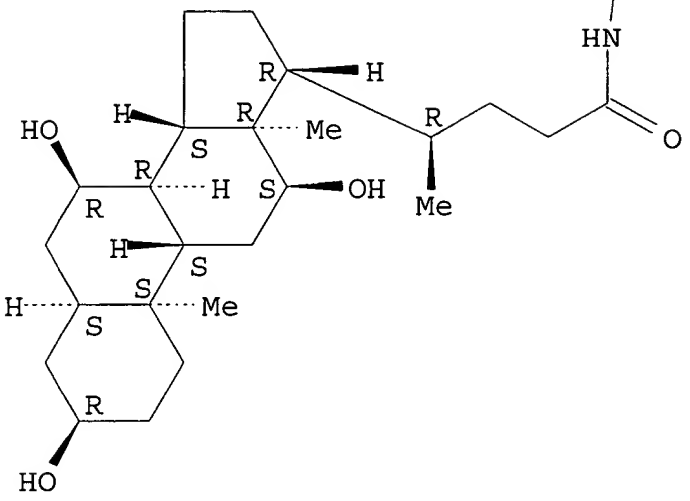

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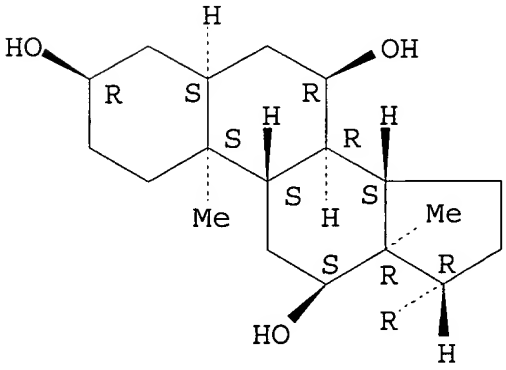

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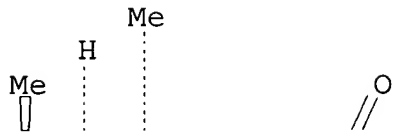
Absolute stereochemistry.

PAGE 1-A



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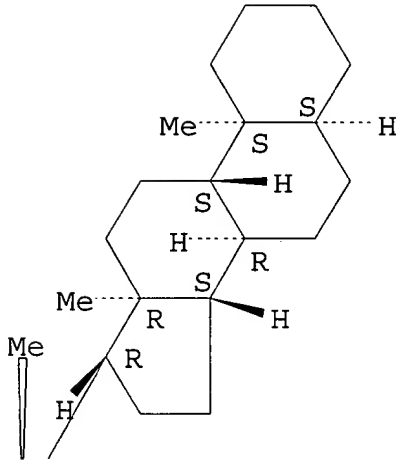

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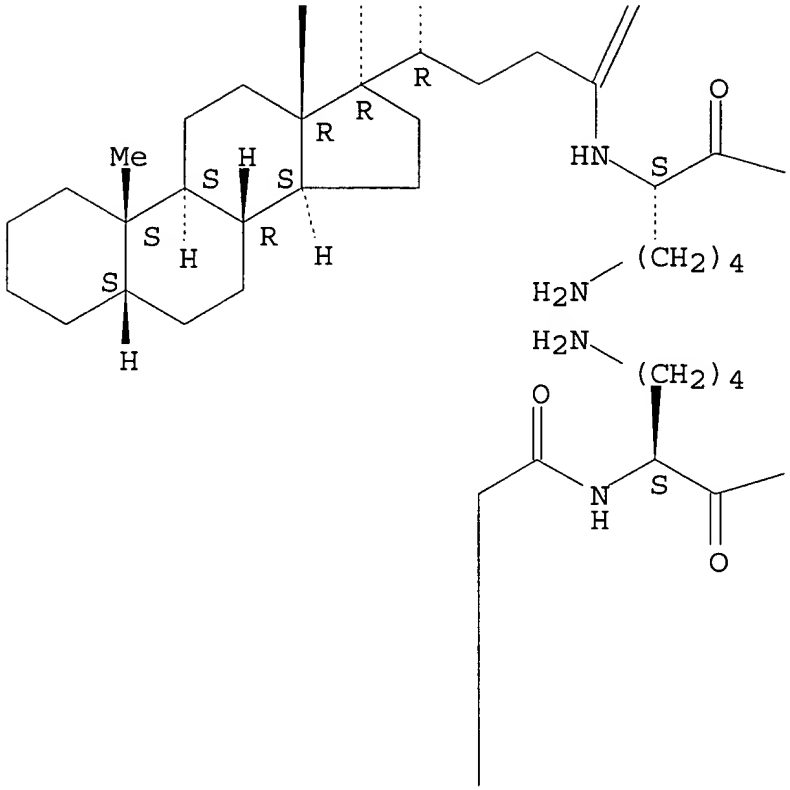

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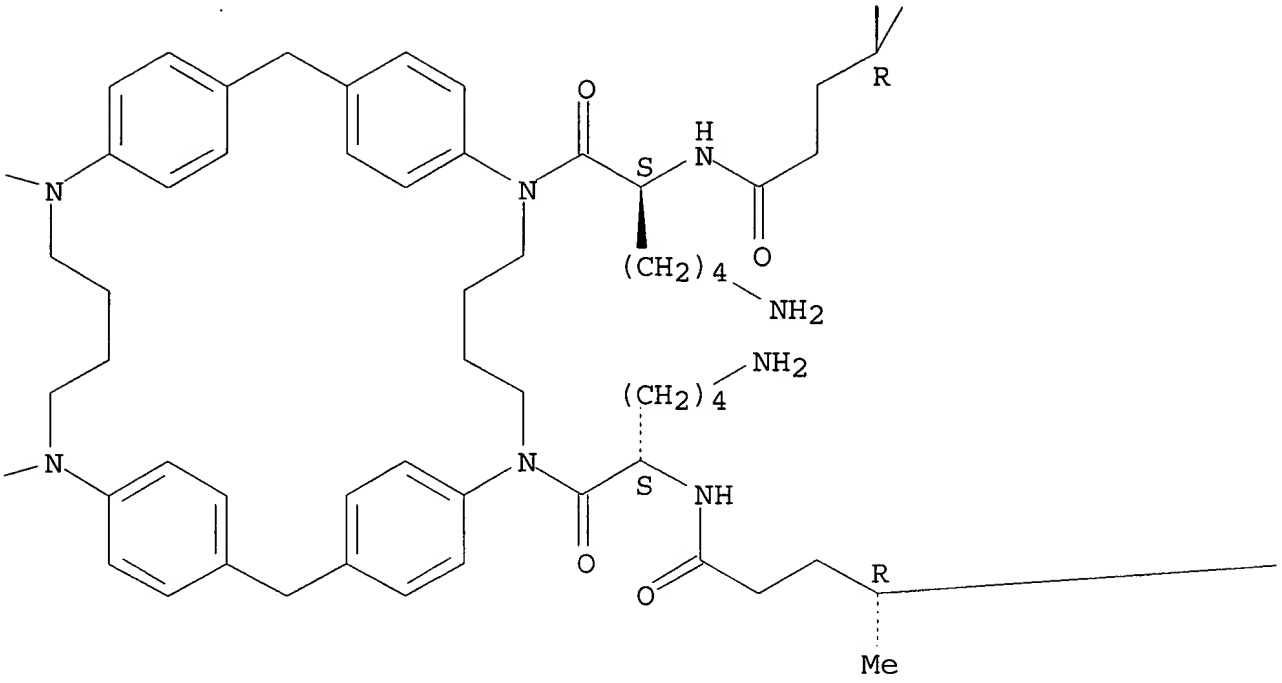

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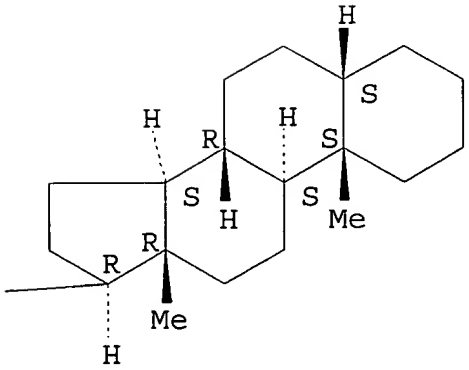

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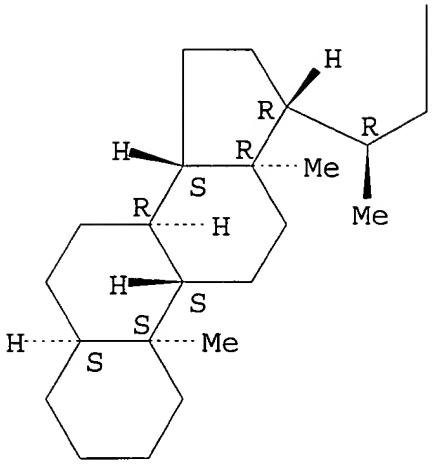

RN 183072-82-4 ZCA
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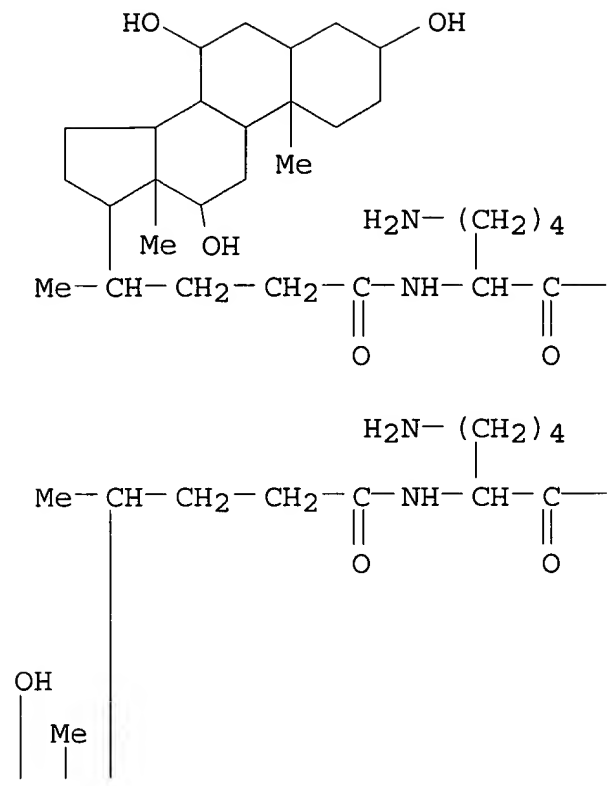
PAGE 1-A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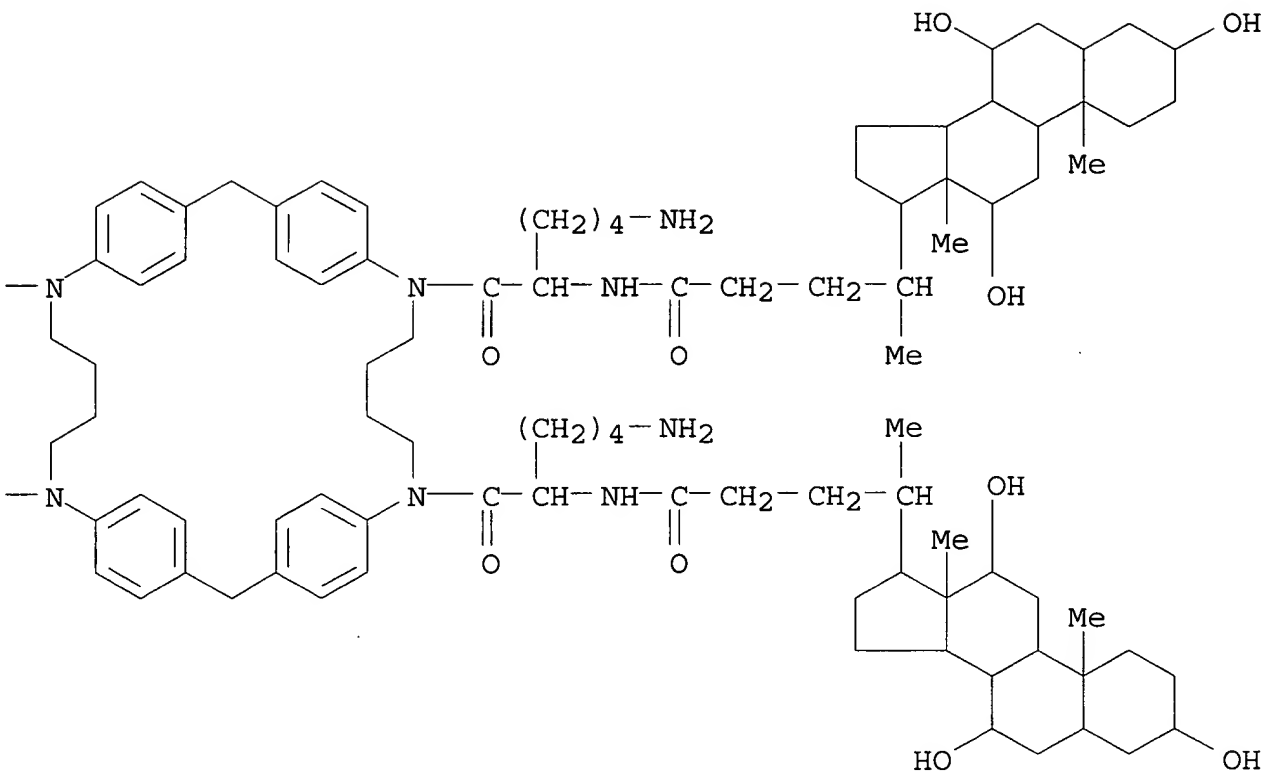
Me
OH
H2N— (CH2)4
Me— CH— CH2— CH2— C— NH— CH— C—
O
O
H2N— (CH2)4
Me— CH— CH2— CH2— C— NH— CH— C—
O
O
OH
Me

PAGE 1-B



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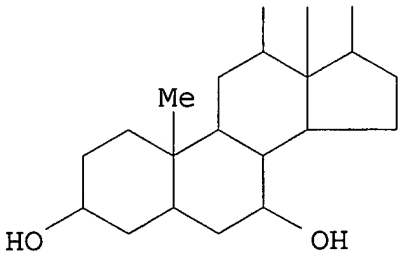
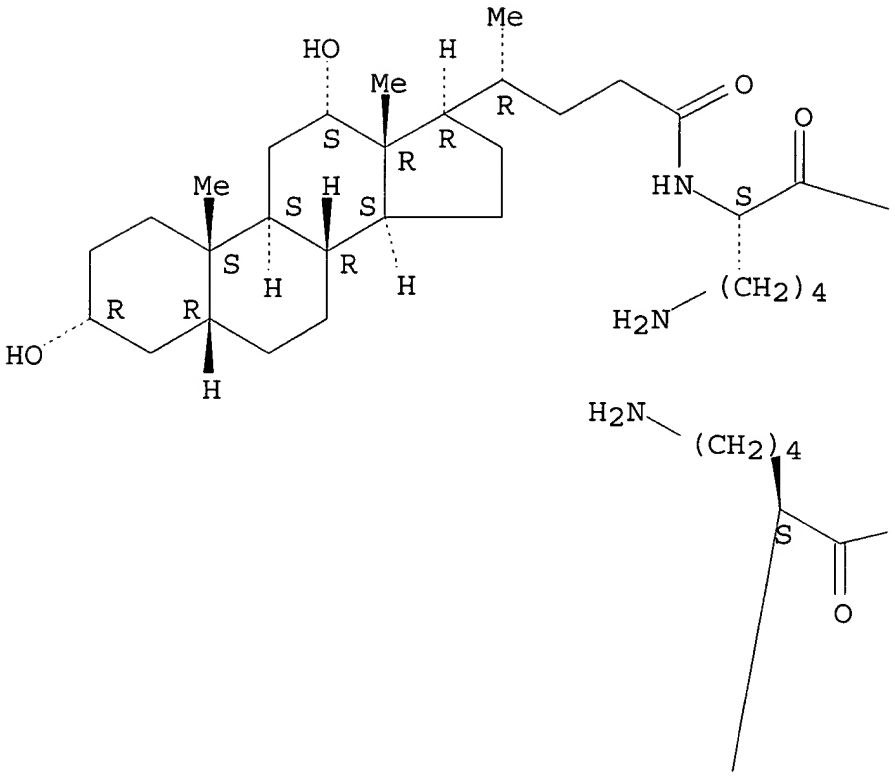


RN 220527-51-5 ZCA
CN Cholan-24-amide, N,N',N'',N'''-[7,12,22,27-tetraazapentacyclo[26.2.2.23,6.213,16.218,21]octatriaconta-3,5,13,15,18,20,28,30,31,33,35,37-dodecaene-7,12,22,27-tetrayltetrakis[(1S)-1-(4-aminobutyl)-2-oxo-2,1-ethanediyl]]tetrakis[3,12-dihydroxy-, (3.alpha.,5.beta.,12.alpha.)-(3'.alpha.,5'.beta.,12'.alpha.)-(3''.alpha.,5''.beta.,12''.alpha.)-(3'''.alpha.,5'''.beta.,12'''.alpha.)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A



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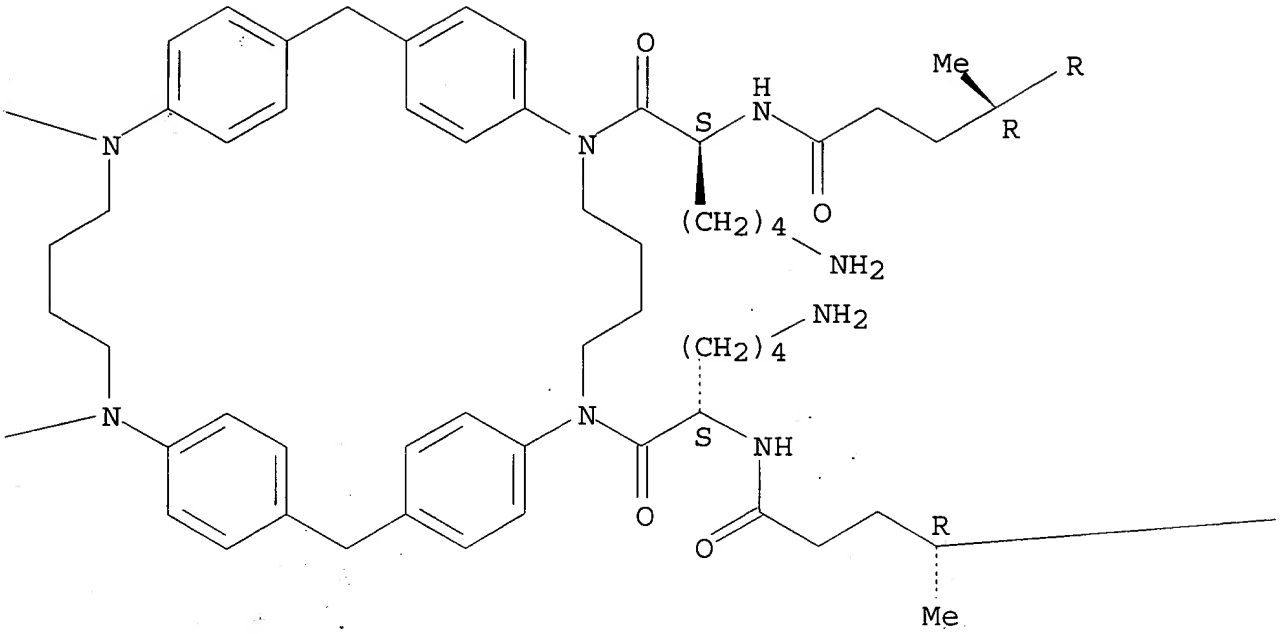

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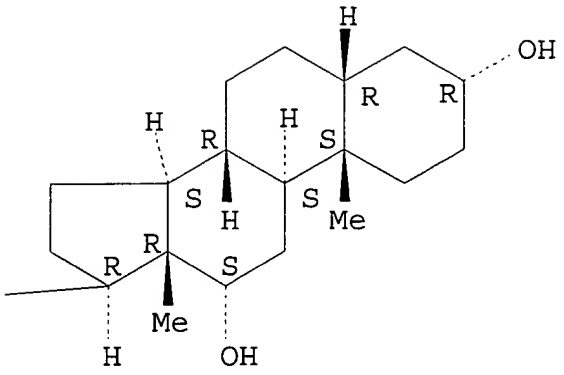

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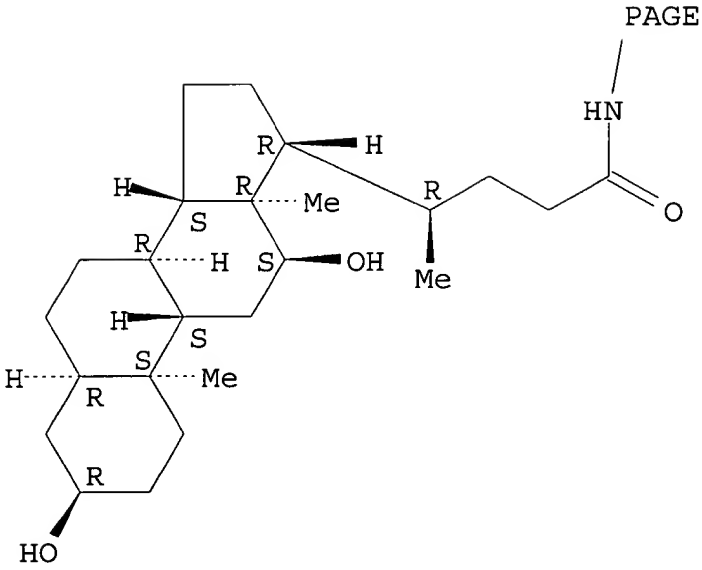

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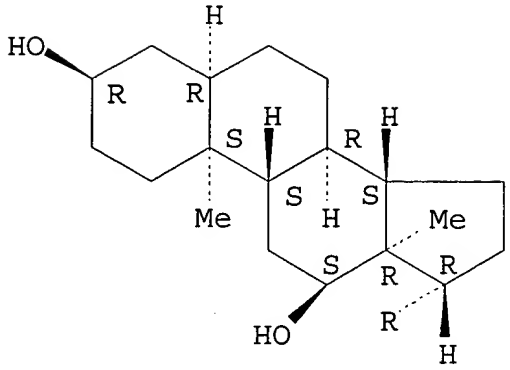

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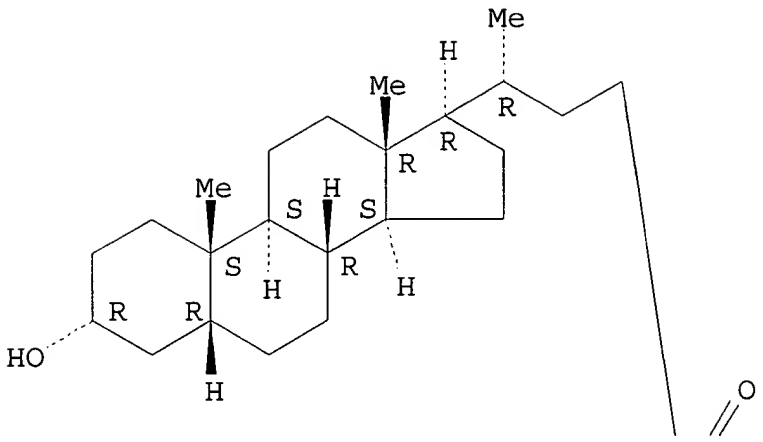
Absolute stereochemistry.

PAGE 1-A



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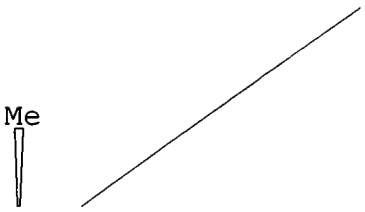

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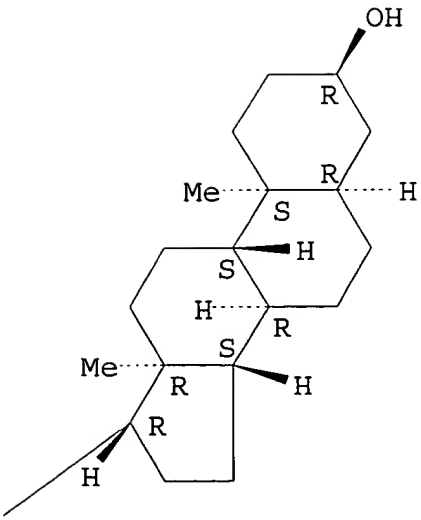

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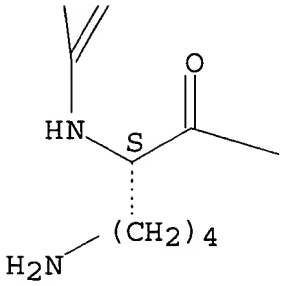

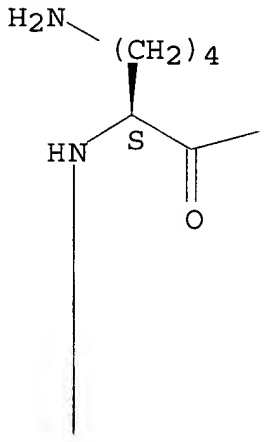

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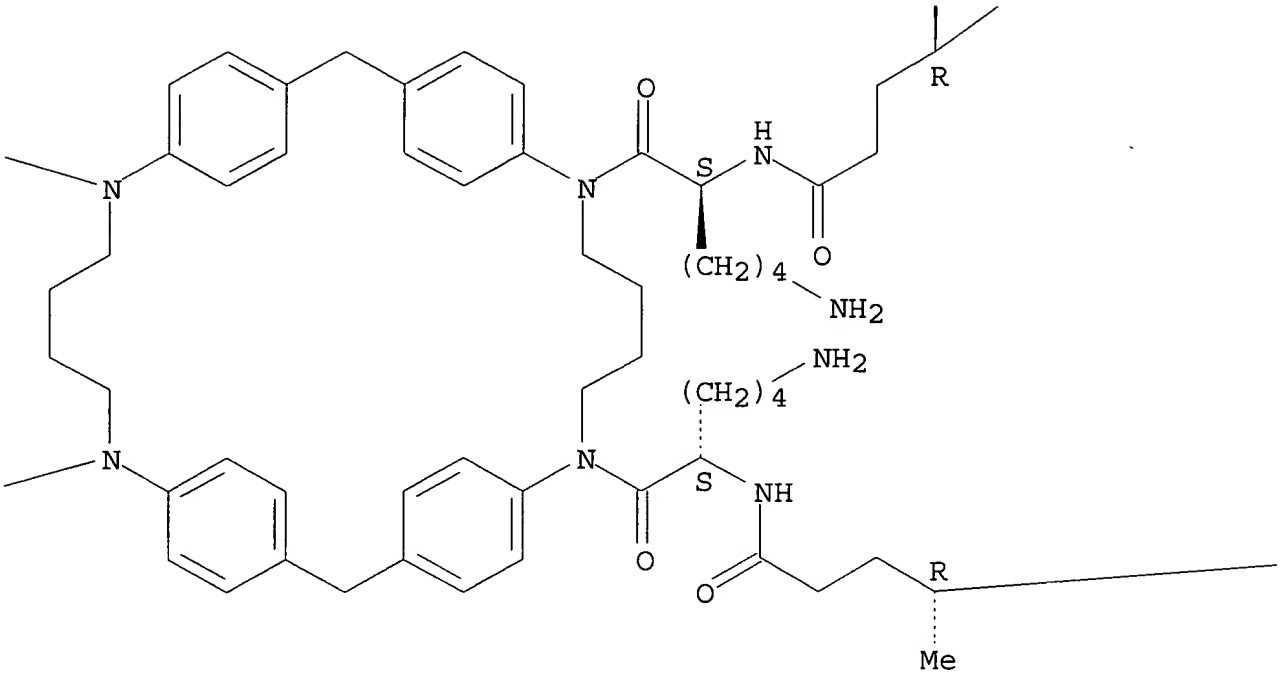

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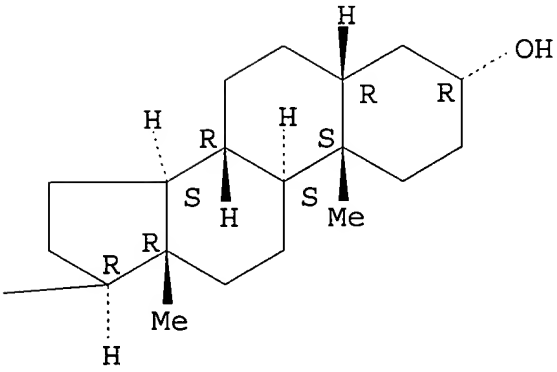

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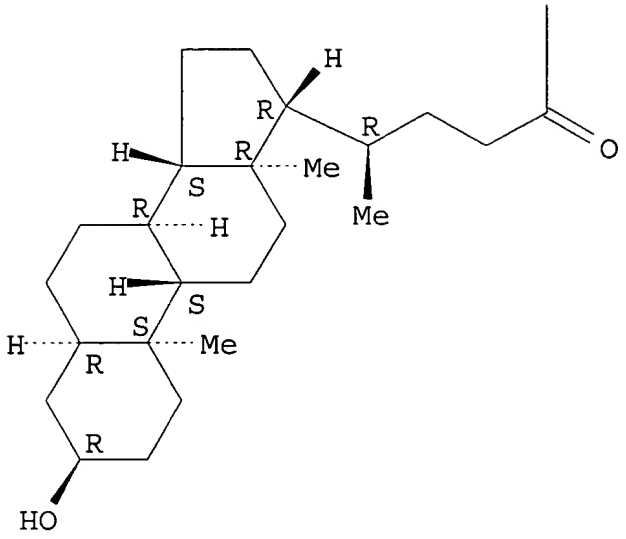


IT **156881-79-7P 182889-23-2P 183072-82-4P**
220527-51-5P 220527-56-0P
(prepn. and characterization of steroid cyclophanes as artificial cell-surface receptors)

L13 ANSWER 11 OF 27 ZCA COPYRIGHT 2003 ACS
127:230718 Characterization of three-dimensionally extended hydrophobic cavities. Difference in molecular recognition ability between steroid and octopus cyclophanes. Kikuchi, Jun-Ichi; Inada, Masahiko; Murakami, Yukito; Egami, Kazuko; Suehiro, Kazuaki (Institute for Fundamental Research in Organic Chemistry, Kyushu University, Fukuoka, 812-81, Japan). Journal of Physical Organic Chemistry, 10(5), 351-357 (English) 1997. CODEN: JPOCEE. ISSN: 0894-3230. Publisher: Wiley.

AB The guest-binding behavior of two different cyclophane hosts, each being capable of providing a three-dimensionally extended hydrophobic cavity toward arom. guests, was examd. in aq. media: a steroid cyclophane bearing four rigid cholate moieties and an octopus cyclophane having four flexible double-chain segments. Even though the binding const. for 2,7-dihydroxynaphthalene with the steroid cyclophane was comparable to that with the octopus cyclophane, the guest binding modes were very different from each other, as confirmed by 1H NMR spectroscopy. I.e., the steroid cyclophane incorporates the guest into its rigid macrocyclic cavity with axial geometry whereas the octopus cyclophane provides a three-dimensional space created by the macrocyclic skeleton and the flexible hydrocarbon chains so that the long axis of the guest becomes more or less perpendicular to the mol. axis of the host upon complexation. Temp.-dependent mol. recognition by these hosts toward 8-anilinonaphthalene-1-sulfonate was examd. by means of fluorescence spectroscopy. Characteristic differences in the guest-binding mode between these hosts were sensitively reflected in

the thermodn. entropy change on host-guest complexation and the temp.-dependent microscopic viscosity experienced by the guest at the binding site.

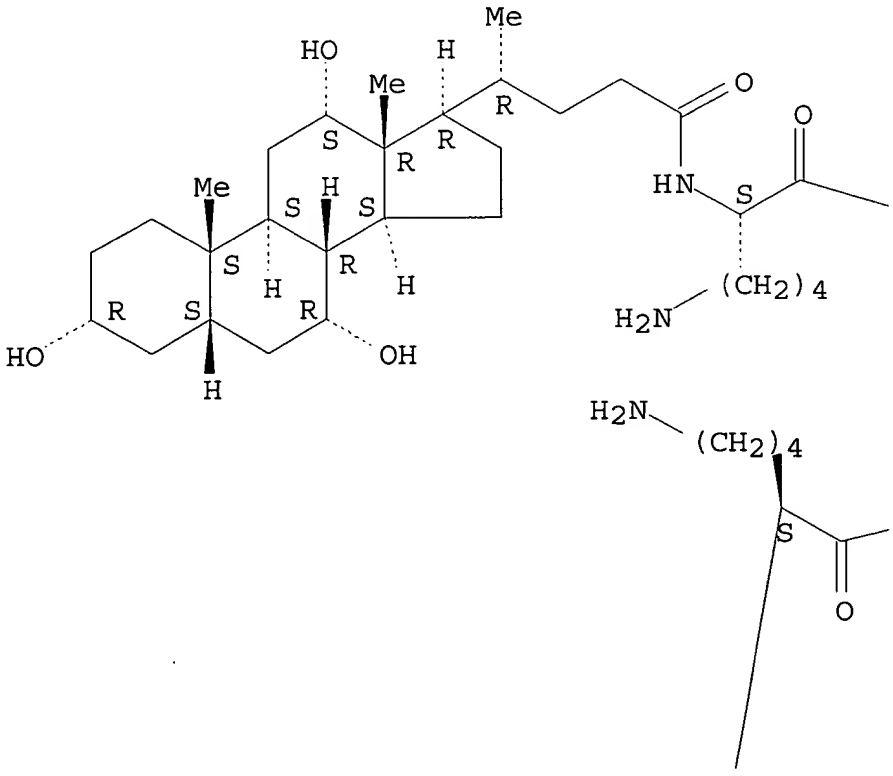
IT **156842-46-5**
(steroid cyclophane incorporates guest into rigid cavity with axial geometry; three-dimensionally extended hydrophobic cavities and difference in mol. recognition ability between steroid and octopus cyclophanes)

RN 156842-46-5 ZCA

CN Cholan-24-amide, N,N',N'',N'''-[7,12,22,27-tetraazapentacyclo[26.2.2.23,6.213,16.218,21]octatriaconta-3,5,13,15,18,20,28,30,31,33,35,37-dodecaene-7,12,22,27-tetrayltetrakis[1-(4-aminobutyl)-2-oxo-2,1-ethanediyl]]tetrakis[3,7,12-trihydroxy-, tetrahydrochloride, stereoisomer (9CI) (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A



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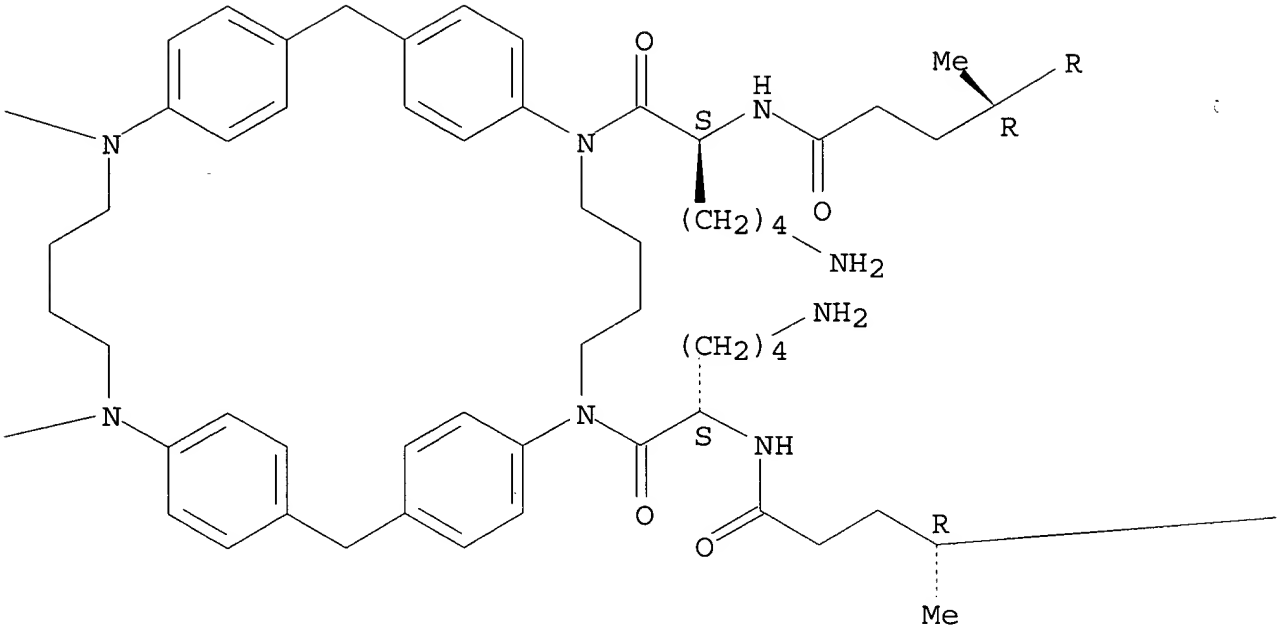

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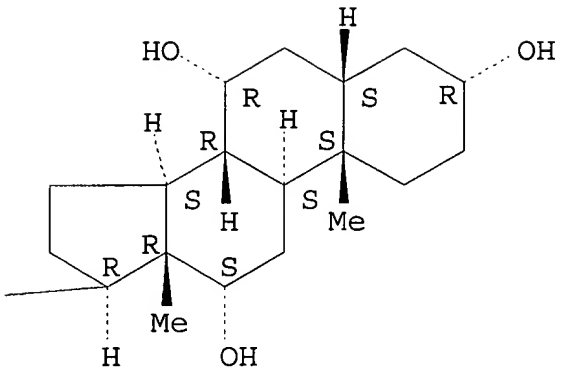

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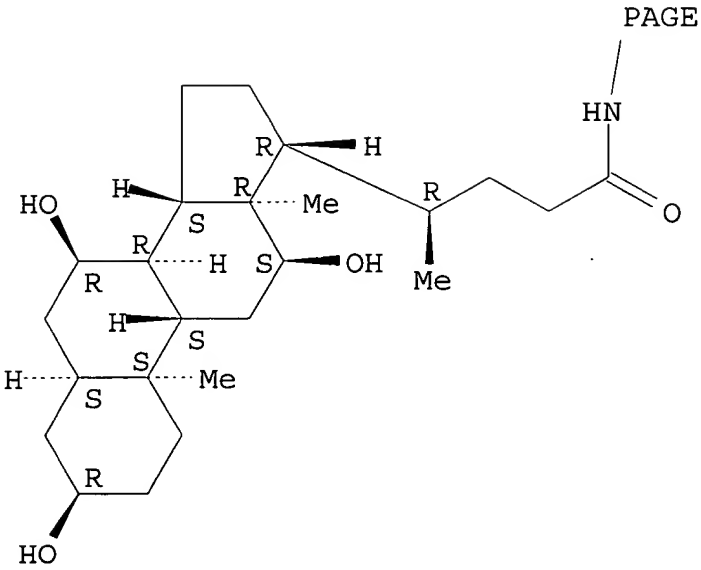
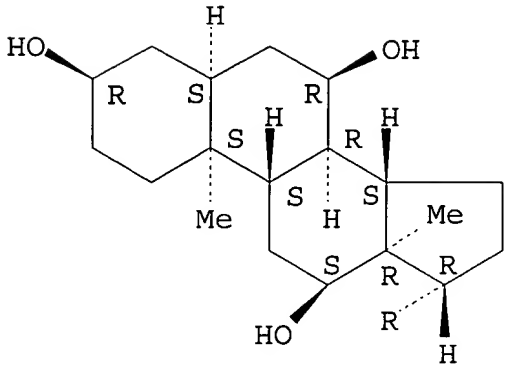


PAGE 3-A



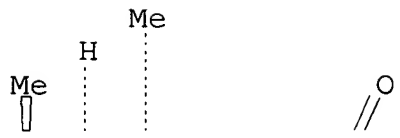
● 4 HCl

IT **156842-46-5**
(steroid cyclophane incorporates guest into rigid cavity with axial geometry; three-dimensionally extended hydrophobic cavities and difference in mol. recognition ability between steroid and octopus cyclophanes)

L13 ANSWER 12 OF 27 ZCA COPYRIGHT 2003 ACS
125:301305 Circular dichroism of an aromatic guest induced by a chiral steroid cyclophane in aqueous solution and synthetic bilayer membrane. Kikuchi, Jun-Ichi; Ogata, Toshiyuki; Inada, Masahiko; Murakami, Yukito (Inst. for Fundamental Res. in Organic Chem., Kyushu Univ., Fukuoka, 812-81, Japan). Chemistry Letters (9), 771-772 (English) 1996. CODEN: CMLTAG. ISSN: 0366-7022. Publisher: Nippon Kagakkai.
AB A steroid cyclophane, having L-lysine residues interposed between a tetraaza[6.1.6.1]paracyclophane skeleton and four cholate moieties, furnished a chiral binding site for a hydrophobic arom. guest in a synthetic bilayer membrane as well as in aq. soln., as evidence by induced CD.
IT **182889-23-2 183072-82-4 183072-83-5 183072-84-6**
(CD of an arom. guest induced by a chiral steroid cyclophane in aq. soln. and synthetic bilayer membrane)
RN 182889-23-2 ZCA
CN Cholan-24-amide, N,N',N'',N'''-[7,12,22,27-tetraazapentacyclo[26.2.2.23,6.213,16.218,21]octatriaconta-3,5,13,15,18,20,28,30,31,33,35,37-dodecaene-7,12,22,27-tetrayltetrakis[1-(4-aminobutyl)-2-oxo-2,1-ethanediyl]]tetrakis-, stereoisomer (9CI) (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A



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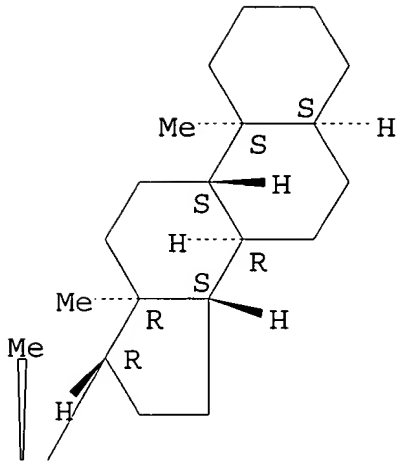

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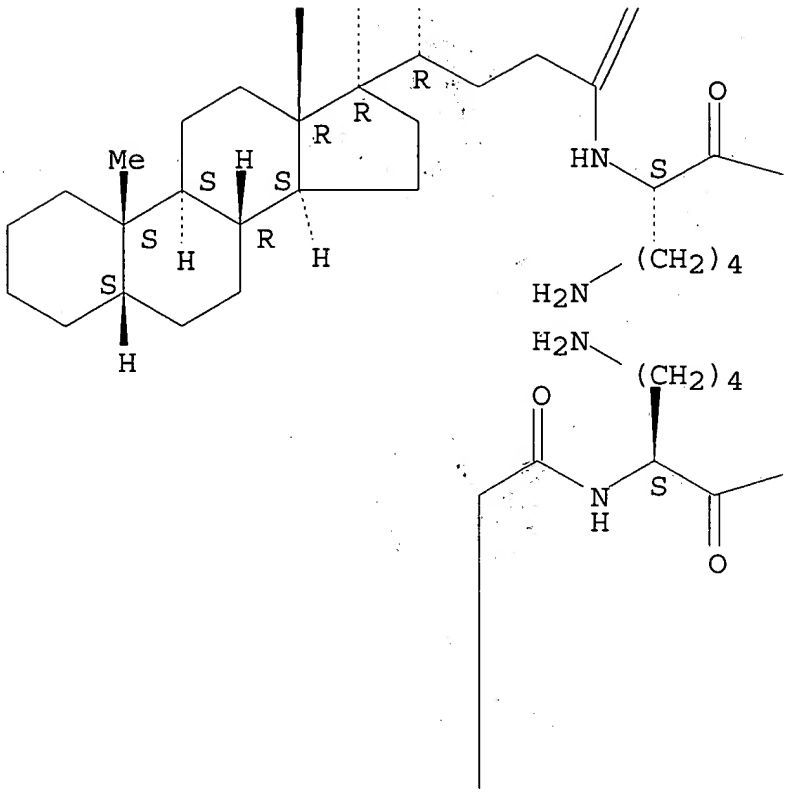
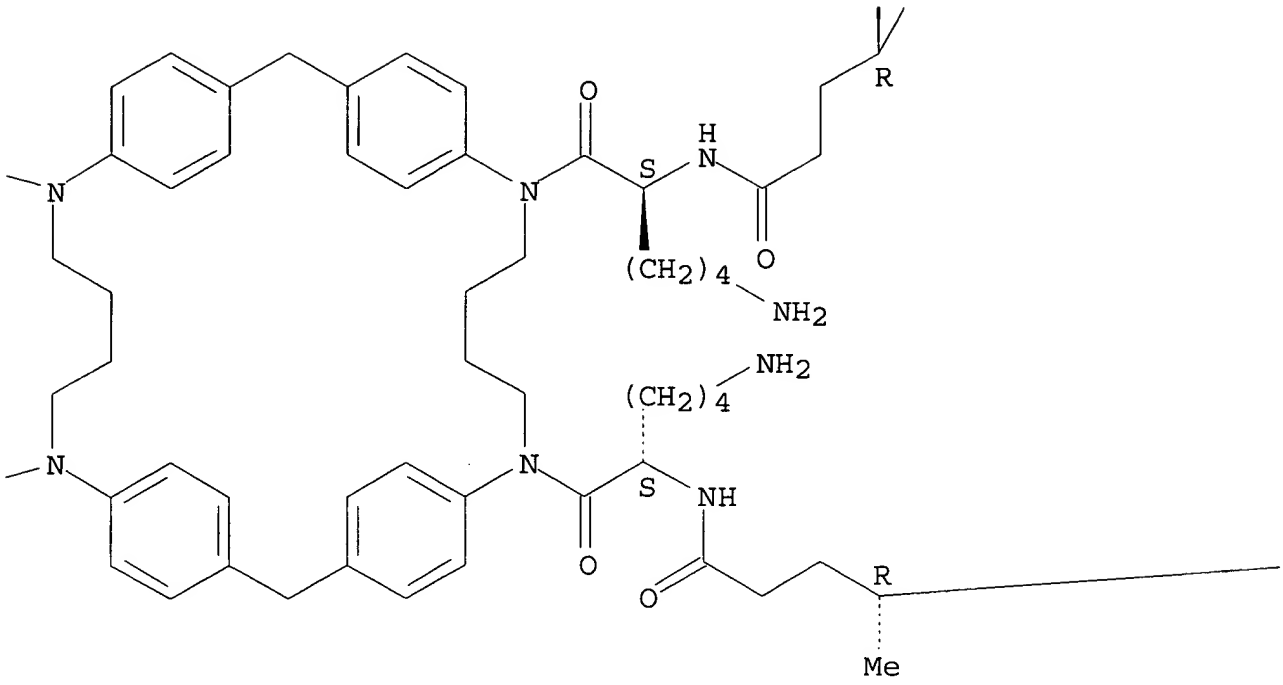


PAGE 2-B



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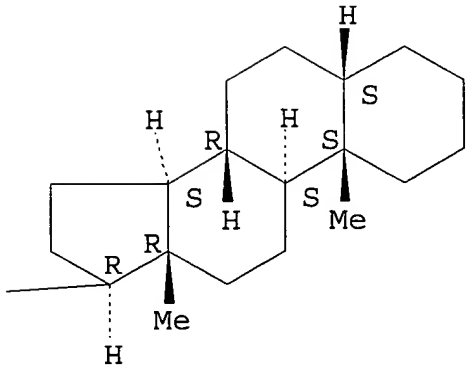

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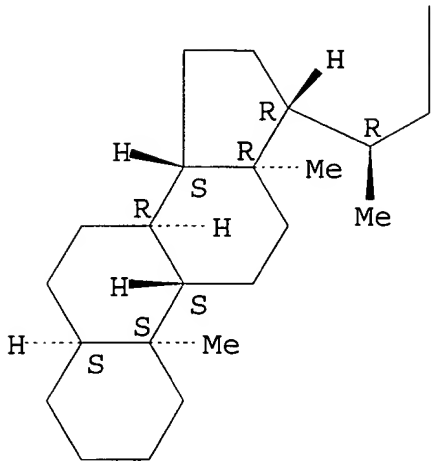

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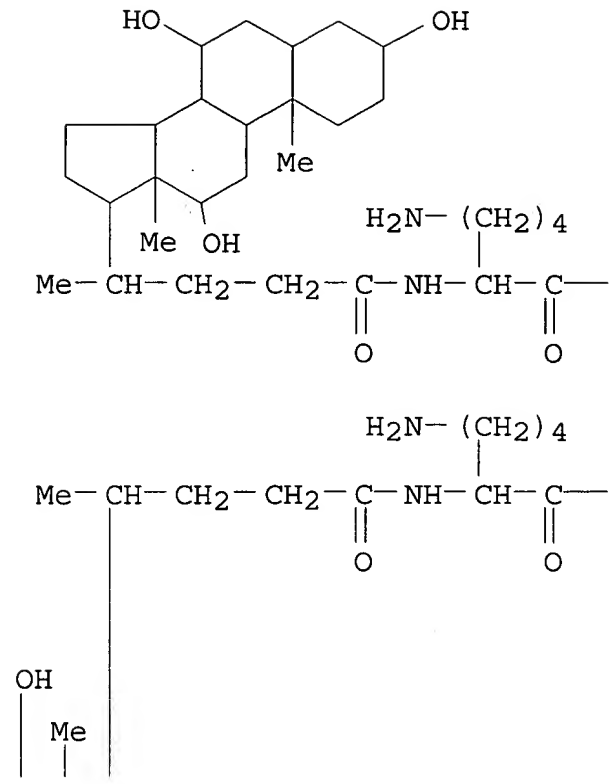
PAGE 1-A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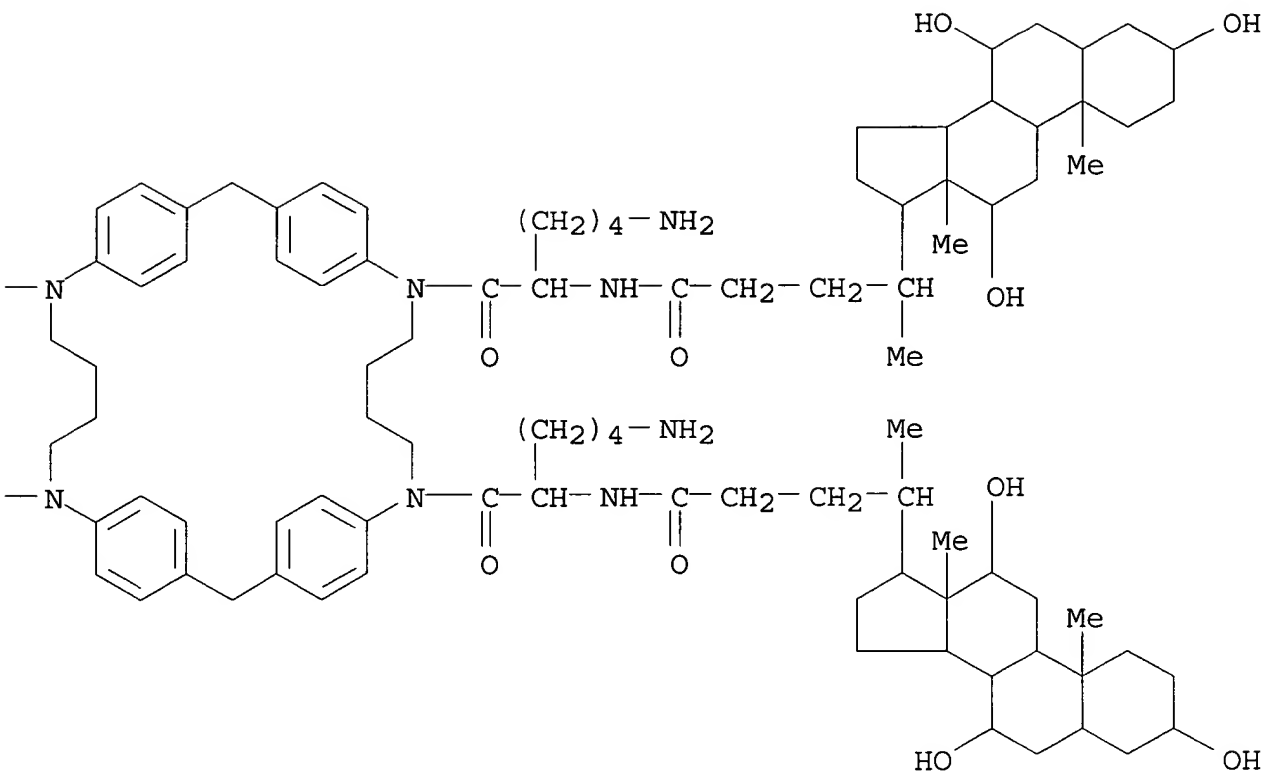
OH
Me
Me
OH
H2N— (CH2)4
Me— CH— CH2— CH2— C— NH— CH— C—
O
O
H2N— (CH2)4
Me— CH— CH2— CH2— C— NH— CH— C—
O
O
OH
Me

PAGE 1-B



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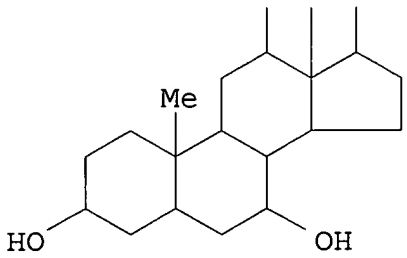
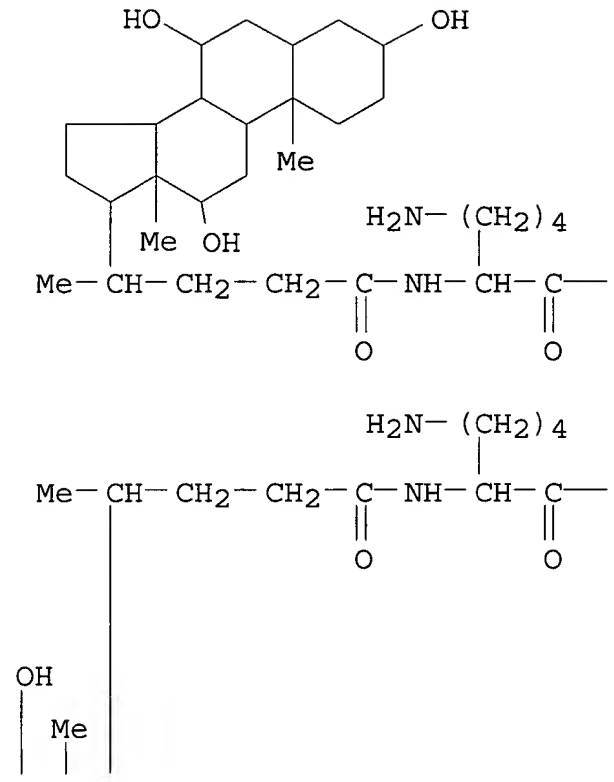


RN 183072-83-5 ZCA
CN Cholan-24-amide, N,N',N'',N'''-[7,12,22,27-tetraazapentacyclo[26.2.2.23,6.213,16.218,21]octatriaconta-3,5,13,15,18,20,28,30,31,33,35,37-dodecaene-7,12,22,27-tetrayltetrakis[1-(4-aminobutyl)-2-oxo-2,1-ethanediyl]]tetrakis[3,7,12-trihydroxy-, stereoisomer, compd. with 6-[(4-methylphenyl)amino]-2-naphthalenesulfonic acid (1:1) (9CI) (CA INDEX NAME)

CM 1

CRN 183072-82-4
CMF C154 H240 N12 O20

PAGE 1-A



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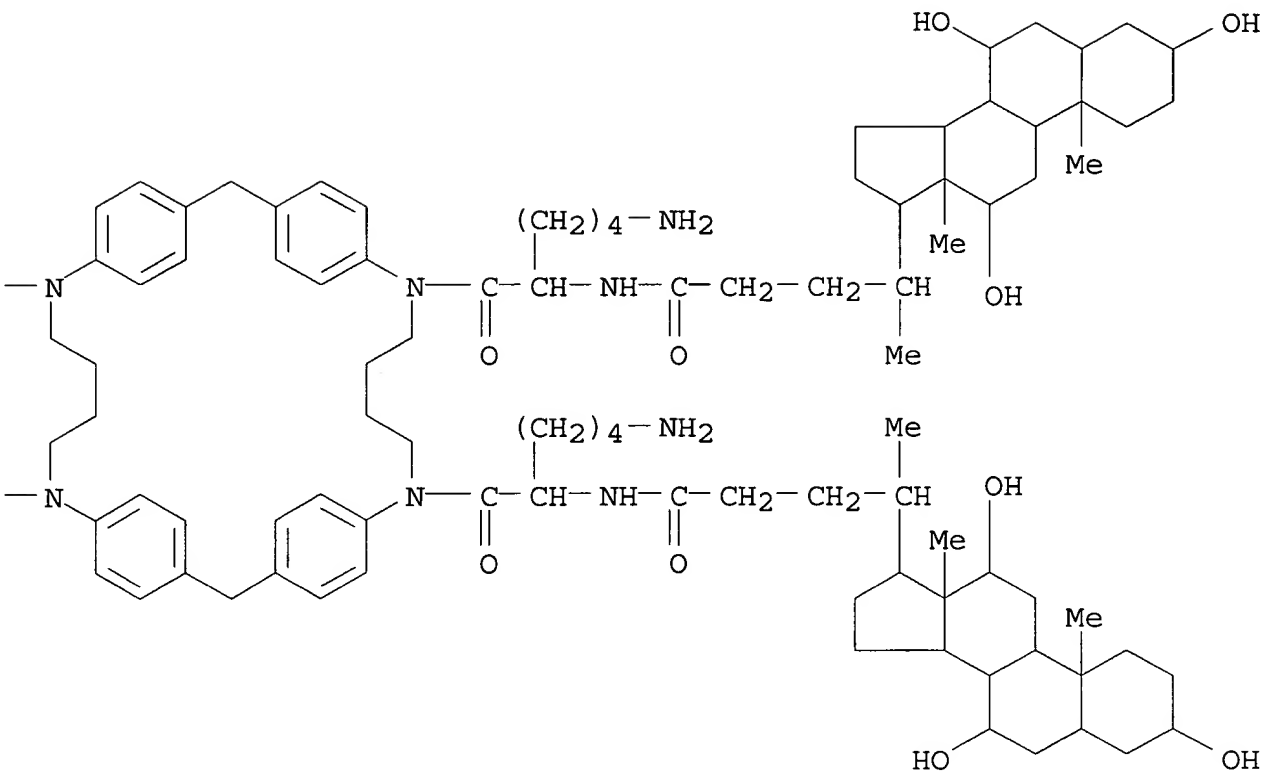

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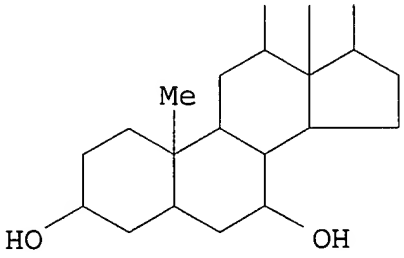
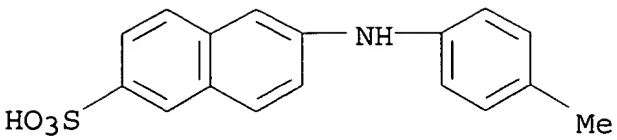


CM 2

CRN 7724-15-4
CMF C17 H15 N O3 S



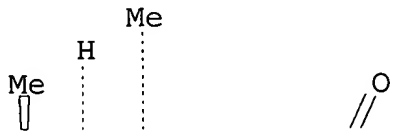
RN 183072-84-6 ZCA
CN Cholan-24-amide, N,N',N'',N'''-[7,12,22,27-tetraazapentacyclo[26.2.2.23,6.213,16.218,21]octatriaconta-3,5,13,15,18,20,28,30,31,33,35,37-dodecaene-7,12,22,27-tetrayltetrakis[1-(4-aminobutyl)-2-oxo-2,1-ethanediyl]]tetrakis-, stereoisomer, compd. with 6-[(4-methylphenyl)amino]-2-naphthalenesulfonic acid (1:1) (9CI) (CA INDEX NAME)

CM 1

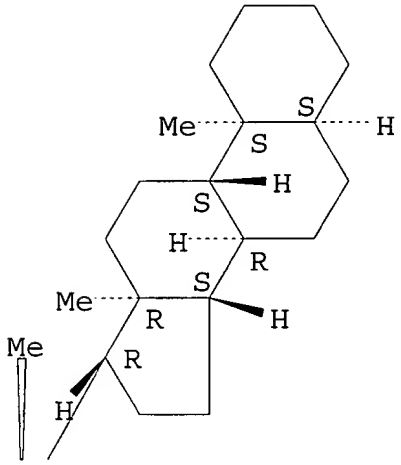
CRN 182889-23-2
CMF C154 H240 N12 O8

Absolute stereochemistry.

PAGE 1-A



PAGE 1-B



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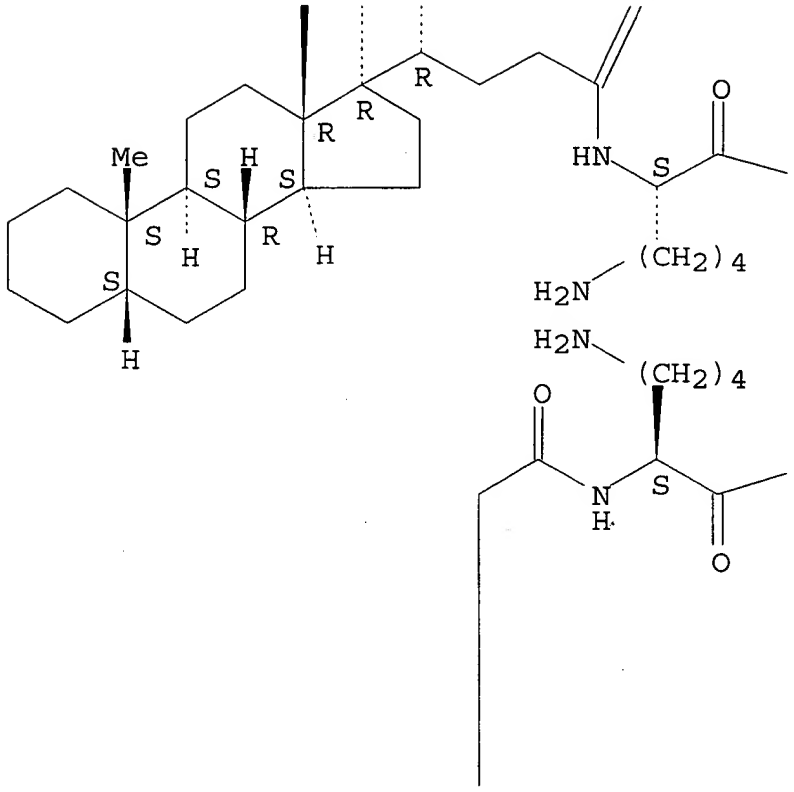

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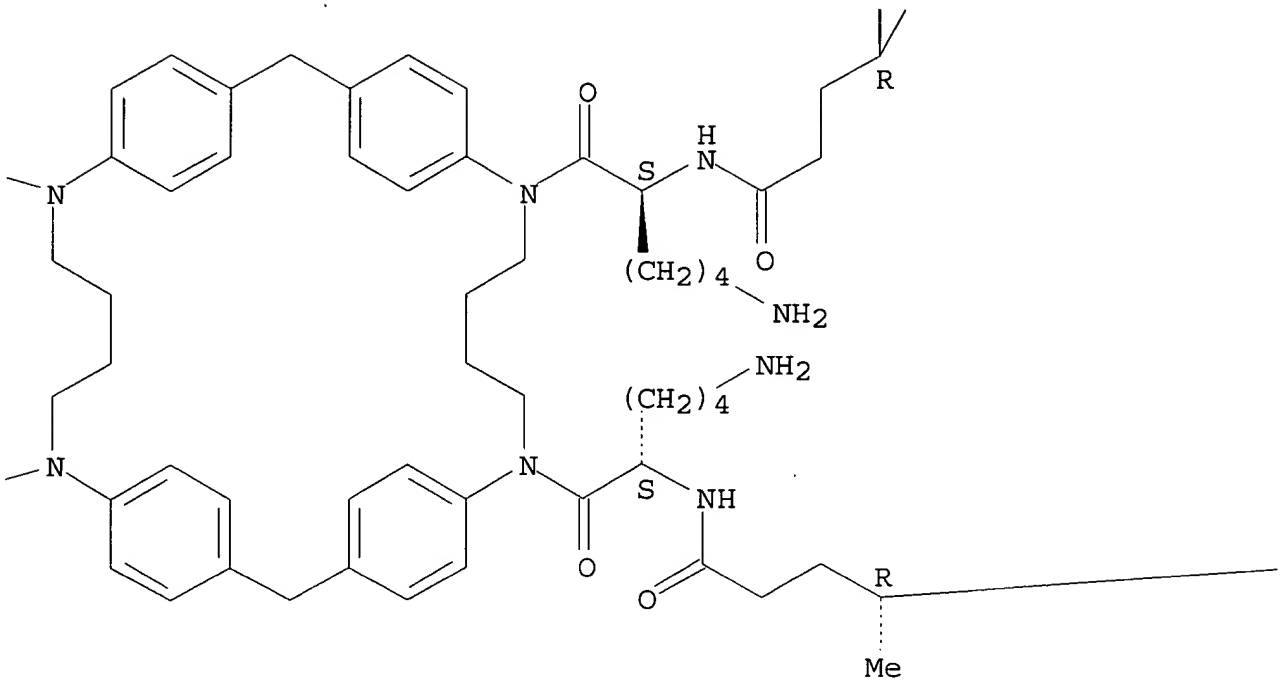

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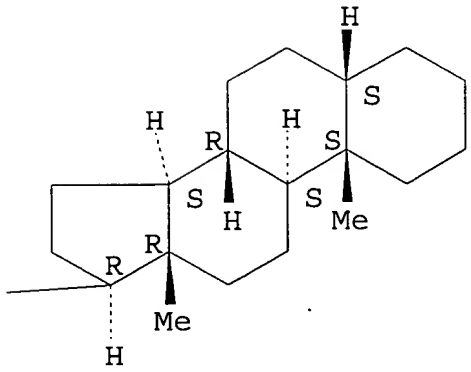

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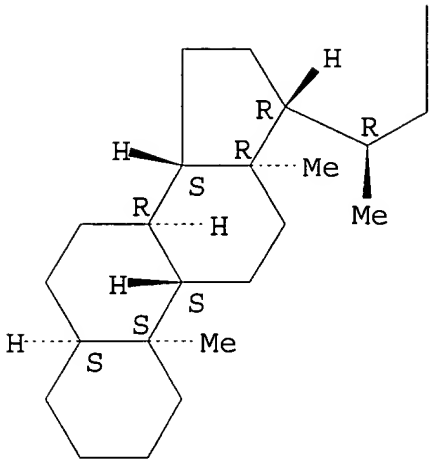

CM 2

CRN 7724-15-4
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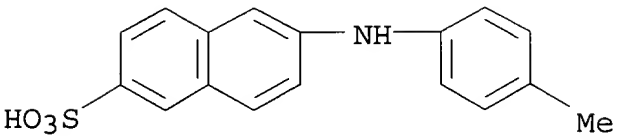
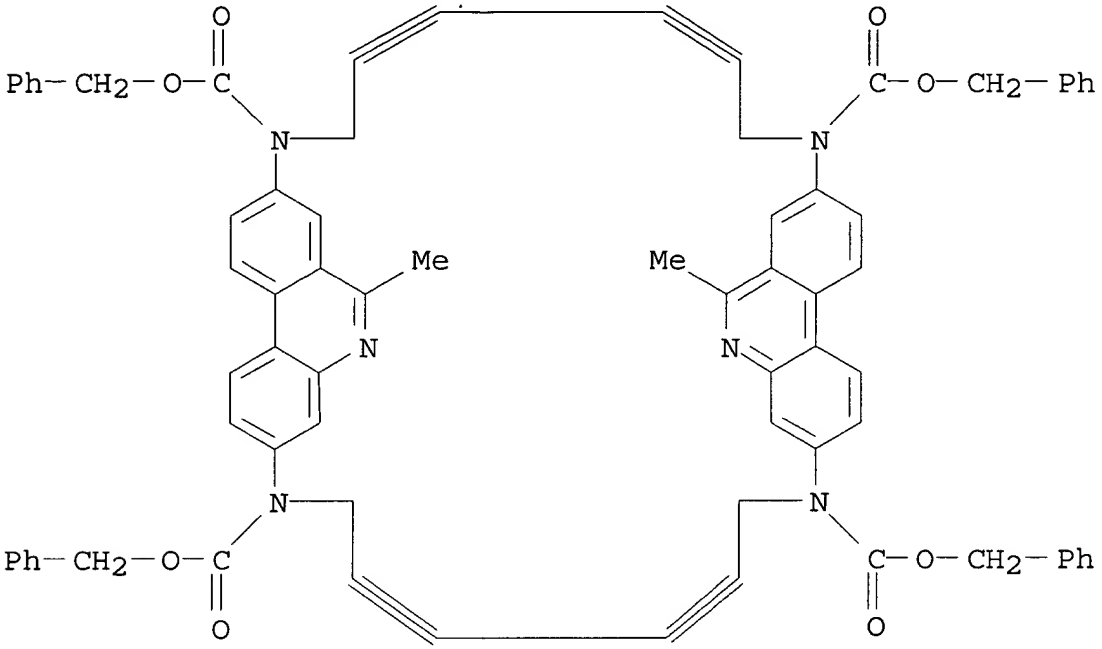


IT **182889-23-2 183072-82-4 183072-83-5**
183072-84-6
(CD of an arom. guest induced by a chiral steroid cyclophane in aq. soln. and synthetic bilayer membrane)

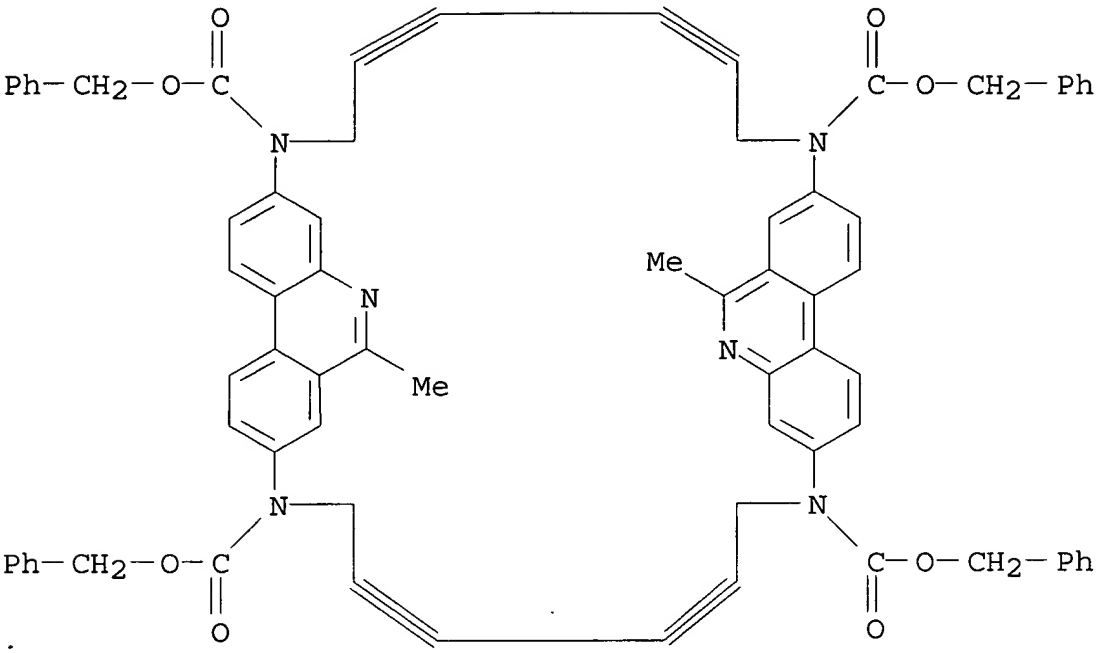
L13 ANSWER 13 OF 27 ZCA COPYRIGHT 2003 ACS
125:221822 Synthesis of cyclo-bis-intercaland receptor molecules with phenanthridinium units. Cudic, Predrag; Zinic, Mladen; Skaric, Vinko; Kiralj, Rudolf; Kojic-Prodic, Biserka; Vigneron, Jean-Pierre; Lehn, Jean-Marie (Lab. Supramol. Nucleoside Chem., Ruder Boskovic Inst., Zagreb, 10000, Croatia). Croatica Chemica Acta, 69(2), 569-611 (English) 1996. CODEN: CCACAA. ISSN: 0011-1643. Publisher: Croatian Chemical Society.
AB The cyclo-bis-intercaland type of receptor mols. based on phenanthridinium units have been synthesized and their spectroscopic (NMR, electronic absorption and fluorescence) properties studied. X-ray structures of two macrocyclic bis-phenanthridine precursors of cyclo-bis-intercalands have been detd.
IT **181584-46-3P 181584-47-4P**
(prepn. of cyclo-bis-intercaland receptor mols. with phenanthridinium units)
RN 181584-46-3 ZCA

CN 1,34:4,7:16,19:22,25-Tetramethenodipyrido[3,4-l:4',3'-b1][1,8,17,24]tetraazacyclodotriacontine-8,15,26,33-tetracarboxylic acid, 10,11,12,13,28,29,30,31-octadehydro-9,14,27,32-tetrahydro-3,20-dimethyl-, tetrakis(phenylmethyl) ester (9CI) (CA INDEX NAME)



RN 181584-47-4 ZCA

CN 1,34:4,7:16,19:22,25-Tetramethenodipyrido[3,4-l:3',4'-b1][1,8,17,24]tetraazacyclodotriacontine-8,15,26,33-tetracarboxylic acid, 10,11,12,13,28,29,30,31-octadehydro-9,14,27,32-tetrahydro-3,21-dimethyl-, tetrakis(phenylmethyl) ester (9CI) (CA INDEX NAME)



IT **181584-46-3P 181584-47-4P**
(prepn. of cyclo-bis-intercaland receptor mols. with phenanthridinium units)

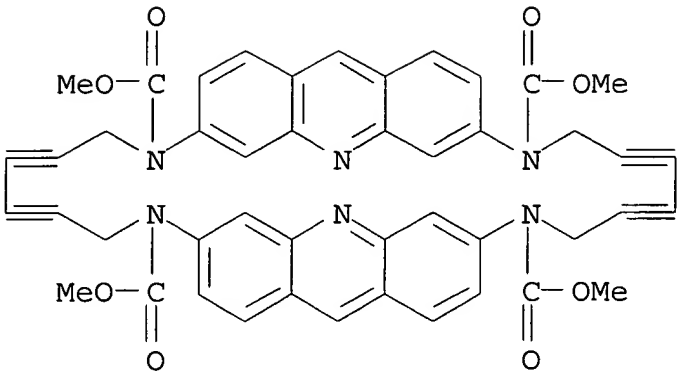
L13 ANSWER 14 OF 27 ZCA COPYRIGHT 2003 ACS
124:117287 Cyclo-bis- and cyclo-tris-intercalands based on acridine subunits. Lorente, Antonio; Fernandez-Saiz, Misericordia; Lehn, Jean-Marie; Vigneron, Jean-Pierre (Dep. quim. Org., Univ. Alcala, Alcala de Henares, 28871, Spain). Tetrahedron Letters, 36(45), 8279-82 (English) 1995. CODEN: TELEAY. ISSN: 0040-4039. Publisher: Elsevier.

AB Macrocyclic receptors contg. proflavine subunits linked by 2,4-hexadiyne spacers have been synthesized. Some physicochem. properties, structural features and cytotoxic activities of these compds. are reported.

IT **173093-90-8P**
(prepn. of cyclo-bis- and cyclo-tris-intercalands based on acridine subunits)

RN 173093-90-8 ZCA

CN 3,6-(Imino[2,4]hexadiynimino[3,6]-endo-acridinoimino[2,4]hexadiynimino)acridine-11,18,29,36-tetracarboxylic acid, tetramethyl ester (9CI) (CA INDEX NAME)



IT **173093-90-8P**
(prepn. of cyclo-bis- and cyclo-tris-intercalands based on acridine subunits)

L13 ANSWER 15 OF 27 ZCA COPYRIGHT 2003 ACS
123:358072 Molecular modeling of host-guest interactions for mass sensitive chemical sensors. Dickert, Franz L.; Reif, Martin; Reif, Hubert (Inst. Analytische Chemie, Univ. Wien, Vienna, A-1090, Austria). Fresenius' Journal of Analytical Chemistry, 352(7-8), 620-4 (English) 1995. CODEN: FJACES. ISSN: 0937-0633. Publisher: Springer.

AB Paracyclophanes are effective coatings for mass sensitive chem. sensors. The enzyme analog recognition can preferably be used to detect arom. and halogenated hydrocarbons. Mol. modeling by the MM3 force field allows the prediction of an efficient analyte inclusion. Besides the necessary steric complementarity it could be shown that the interaction between the Me groups of arom. guests (e.g. toluene) and the arom. walls of the host is essential for host-guest complexation. These phenomena get more pronounced if bicyclic cyclophanes are applied and these sensitive materials enable the detection of only a few ppm of toluene with SAW devices. Also, the electron-rich di-Ph ether moieties of these hosts guarantee interactions with electron-deficiency analytes such as chlorinated hydrocarbons with a selectivity superior to that of the monocyclic materials.

IT **171192-86-2**
(mol. modeling of host-guest interactions for mass sensitive chem. sensors)

RN 171192-86-2 ZCA
CN 10,28,43-Trioxa-5,15,23,33,38,48-hexaazadecacyclo[17.17.13.26,9.211,14.224,27.229,32.239,42.244,47.13,35.117,21]trihexaconta-1,3(54),6,8,11,13,17,19,21(59),24,26,29,31,35,39,41,44,46,50,52,55,57,60,62-tetracosaene, 5,15,23,33,38,48-hexamethyl- (9CI) (CA INDEX NAME)

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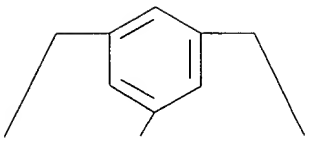

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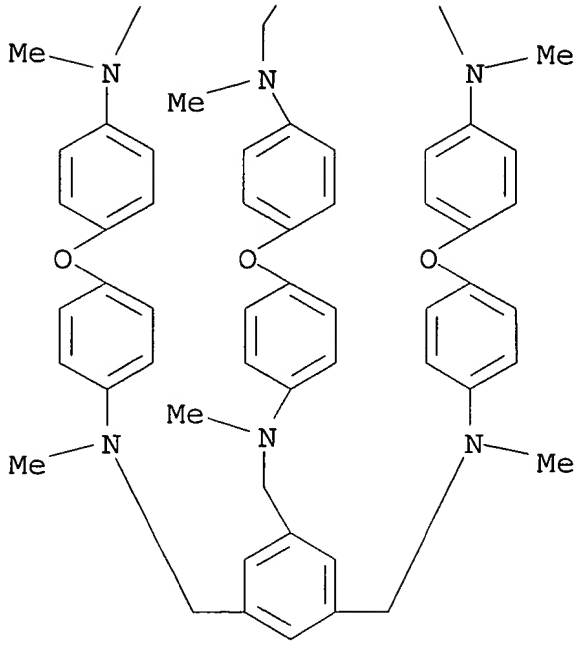
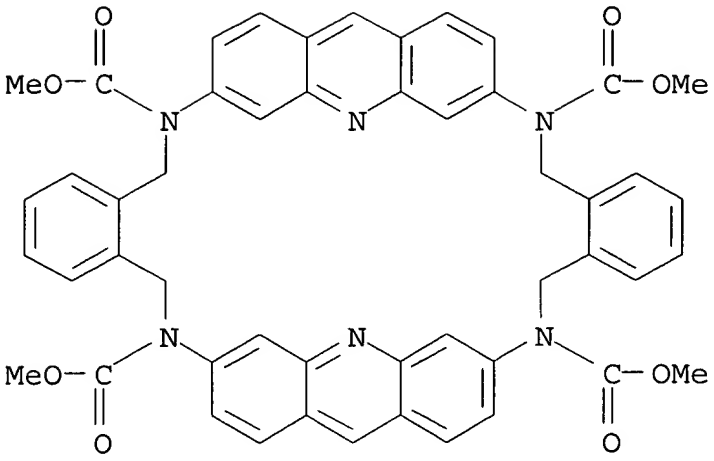
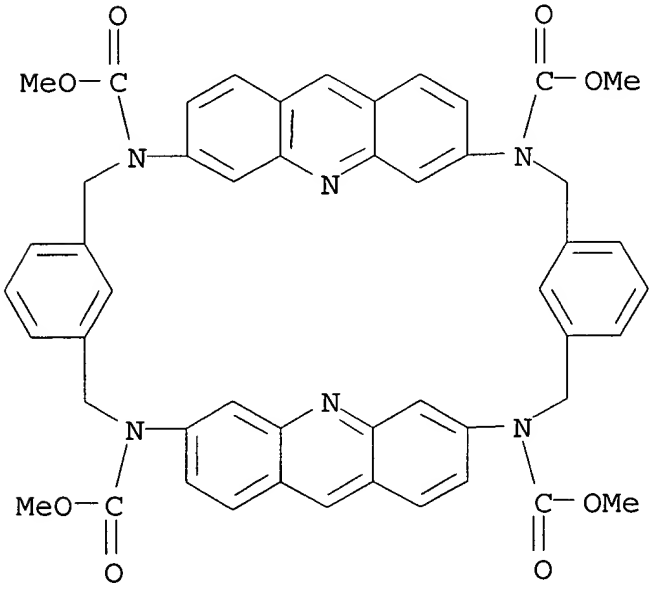


IT **171192-86-2**
(mol. modeling of host-guest interactions for mass sensitive chem. sensors)

L13 ANSWER 16 OF 27 ZCA COPYRIGHT 2003 ACS
123:313904 Cyclo-bis-intercalands with acridine subunits linked by rigid spacers. Lorente, Antonio; Fernandez-Saiz, Misericordia; Espinosa, Juan-Felix; Jaime, Carlos; Lehn, Jean-Marie; Vigneron, Jean-Pierre (Dep. Quim. Org., Univ. Alcala, Alcala de Henares, Spain). Tetrahedron Letters, 36(29), 5261-4 (English) 1995. CODEN: TELEAY. ISSN: 0040-4039. Publisher: Elsevier.
AB Tweezer and macrocyclic compds. contg. two acridine subunits have been synthesized. A structural study by spectroscopic and mol. mechanics methods is reported. The in vitro cytotoxicity of some of the compds. was evaluated.
IT **170302-02-0P 170302-03-1P**
(prepn. of bis-intercalands with acridine subunits linked by rigid spacers)
RN 170302-02-0 ZCA
CN 7,11:10,14:13,17:26,30:29,33:32,36-Hexamethenodibenzo[c,t][1,6,12,18,23,29]hexaazacyclotetratriacontine-6,18,25,37-tetracarboxylic acid, 5,19,24,38-tetrahydro-, tetramethyl ester (9CI) (CA INDEX NAME)



RN 170302-03-1 ZCA
CN 3,6-(Iminomethano[1,3]benzenomethanimino[3,6]-endo-acridinoiminomethano[1,3]benzenomethanimino)acridine-11,20,31,40-tetracarboxylic acid, tetramethyl ester (9CI) (CA INDEX NAME)



IT **170302-02-0P 170302-03-1P**
(prepn. of bis-intercalands with acridine subunits linked by rigid spacers)

L13 ANSWER 17 OF 27 ZCA COPYRIGHT 2003 ACS
123:227785 The binding properties of cyclophane dimers. Breslow, Ronald; Duggan, Peter J.; Wiedenfeld, David; Waddell, Sherman T. (Dep. Chem., Columbia Univ., New York, NY, 10027, USA). Tetrahedron Letters, 36(16), 2707-10 (English) 1995. CODEN: TELEAY. ISSN:

0040-4039. OTHER SOURCES: CASREACT 123:227785. Publisher: Elsevier.

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* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

AB Two water sol. cyclophane dimers have been prepd., and their binding properties examd. With a range of bidentate guests, the affinities of the new dimeric cyclophanes were similar to those of the monomeric analog. The alc. I was treated with thioxanthone-3,6-dicarbonyl dichloride, Et3N, DMAP and ClCH2CH2Cl to give a product which was converted to the dimer II. Binding consts. (25.degree.) in water showed that II had a higher affinity for bidentate guest than for monodentate analogs.

IT **168427-05-2P 168427-08-5P**
(the binding properties of cyclophane dimers)

RN 168427-05-2 ZCA

CN 9H-Thioxanthene-3,6-dicarboxylic acid, 9-oxo-, bis(7,13,23,29-tetramethyl-7,13,23,29-tetraazapentacyclo[28.2.2.23,6.214,17.219,22]tetraconta-3,5,14,16,19,21,30,32,33,35,37,39-dodecaene-10,10'-diyl) ester (9CI) (CA INDEX NAME)

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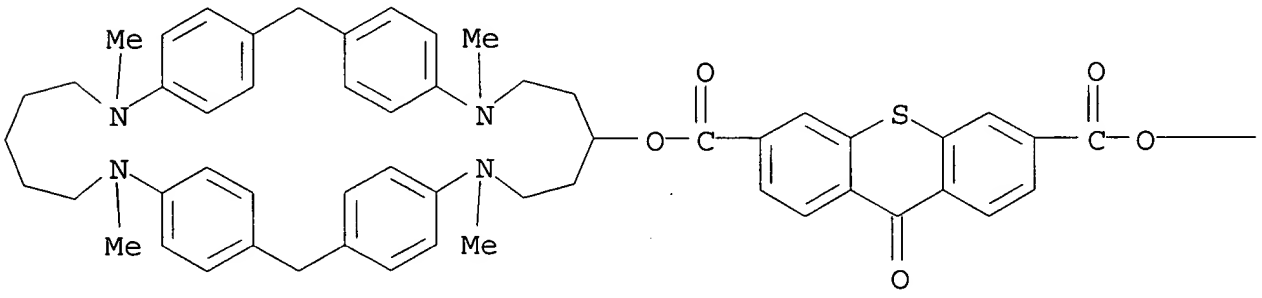
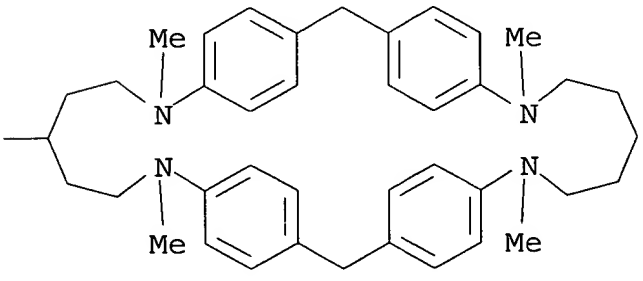


PAGE 1-B



RN 168427-08-5 ZCA
CN 1,4-Benzenedicarboxamide, N,N'-bis(7,13,23,29-tetramethyl-7,13,23,29-tetraazapentacyclo[28.2.2.23,6.214,17.219,22]tetraconta-3,5,14,16,19,21,30,32,33,35,37,39-dodecaen-10-yl)- (9CI) (CA INDEX NAME)

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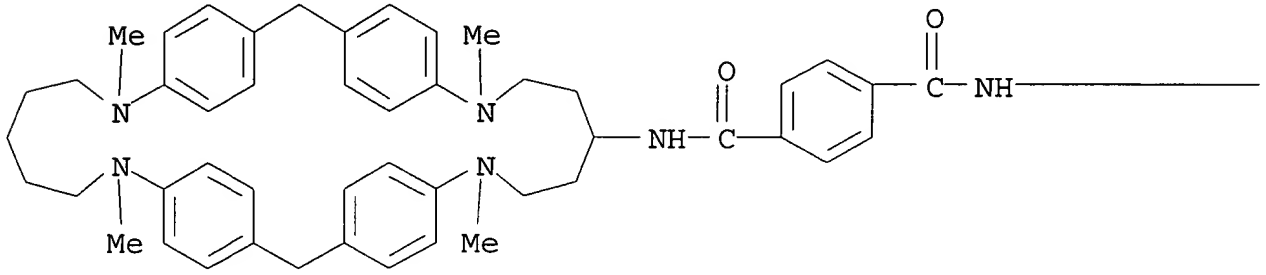
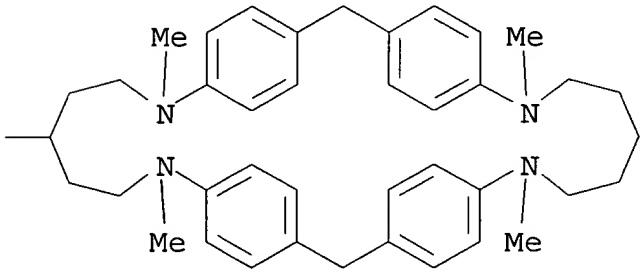
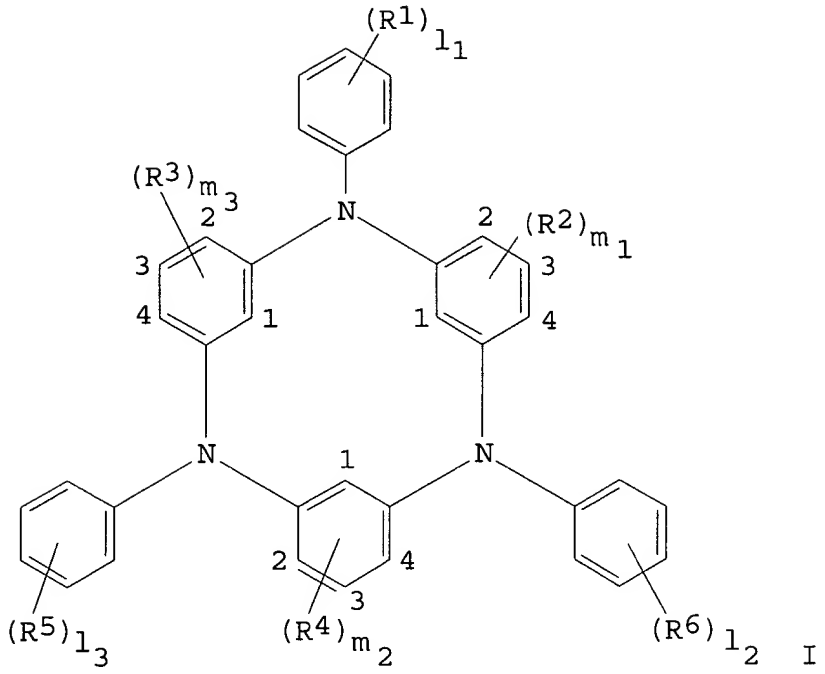


PAGE 1-B



IT **168427-05-2P 168427-08-5P**
(the binding properties of cyclophane dimers)

L13 ANSWER 18 OF 27 ZCA COPYRIGHT 2003 ACS
121:289574 Electrophotographic photoreceptor. Hayata, Hirofumi (Konishiroku Photo Ind, Japan). Jpn. Kokai Tokkyo Koho JP 05323635 A2 19931207 Heisei, 17 pp. (Japanese). CODEN: JKXXAF. APPLICATION: JP 1992-128796 19920521.
GI

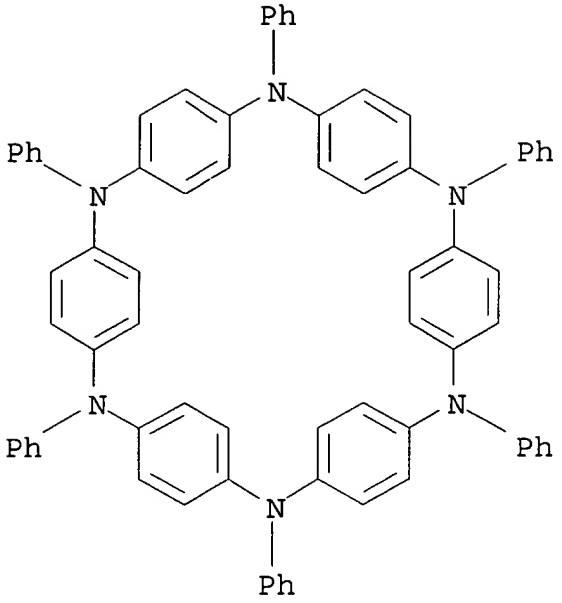


AB The title electrophotog. photoreceptor has a photosensitive layer contg. a cyclic triphenylamine, for example I (R1-6 = H, halo, alkyl, alkoxy, aryl, alkylamino; l1-3 = 0-5; m1-3 = 0-4). The photoreceptor shows superior chargeability, high-sensitivity, and durability.

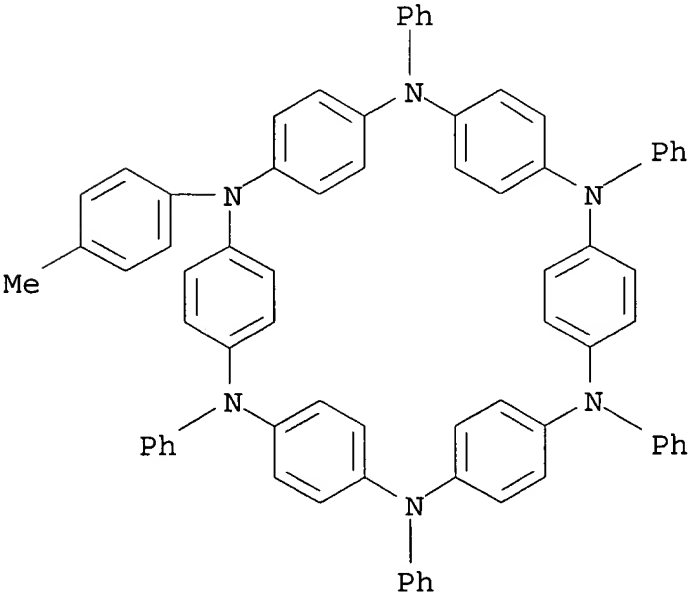
IT **157914-30-2 157914-31-3 157914-32-4**
157914-33-5 157914-34-6 157914-35-7
157914-36-8 157914-37-9 157914-38-0
157914-39-1 157914-40-4
(electrophotog. photoreceptor using)

RN 157914-30-2 ZCA

CN 2,7,12,17,22,27-Hexaazaheptacyclo[26.2.2.23,6.28,11.213,16.218,21.223,26]dotetraconta-3,5,8,10,13,15,18,20,23,25,28,30,31,33,35,37,39,41-octadecaene, 2,7,12,17,22,27-hexaphenyl- (9CI) (CA INDEX NAME)

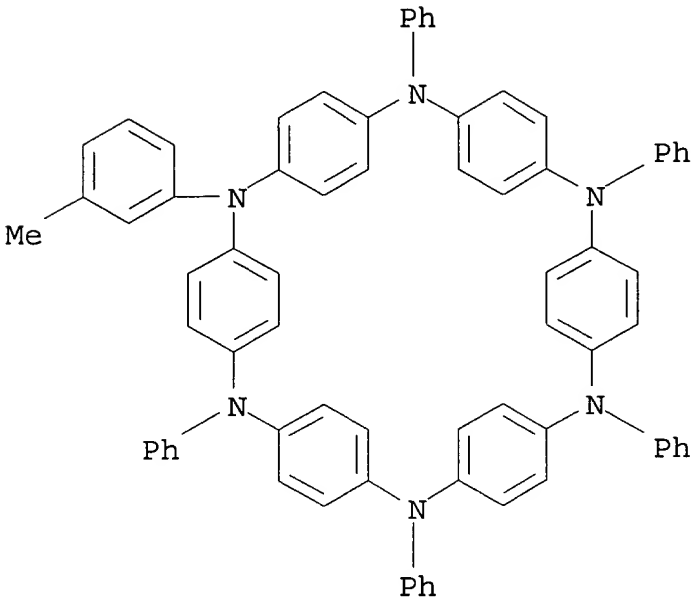


RN 157914-31-3 ZCA
CN 2,7,12,17,22,27-Hexaazaheptacyclo[26.2.2.23,6.28,11.213,16.218,21.223,26]dotetraconta-3,5,8,10,13,15,18,20,23,25,28,30,31,33,35,37,39,41-octadecaene, 2-(4-methylphenyl)-7,12,17,22,27-pentaphenyl- (9CI) (CA INDEX NAME)

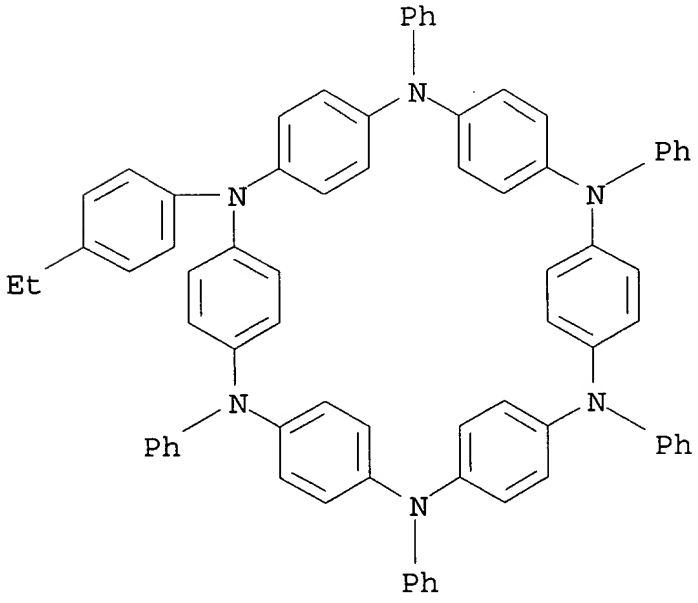


RN 157914-32-4 ZCA
CN 2,7,12,17,22,27-Hexaazaheptacyclo[26.2.2.23,6.28,11.213,16.218,21.223,26]dotetraconta-3,5,8,10,13,15,18,20,23,25,28,30,31,33,35,37,39,41-

octadecaene, 2-(3-methylphenyl)-7,12,17,22,27-pentaphenyl- (9CI) (CA INDEX NAME)

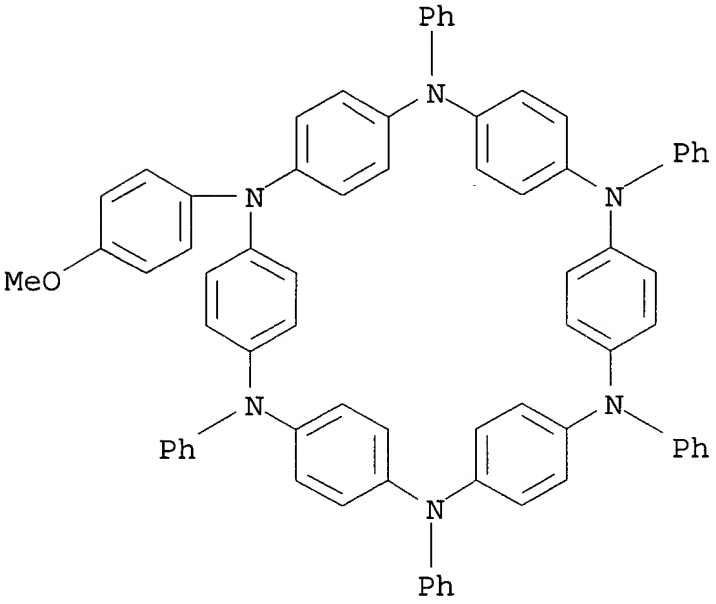


RN 157914-33-5 ZCA
CN 2,7,12,17,22,27-Hexaazaheptacyclo[26.2.2.23,6.28,11.213,16.218,21.223,26]dotetraconta-3,5,8,10,13,15,18,20,23,25,28,30,31,33,35,37,39,41-octadecaene, 2-(4-ethylphenyl)-7,12,17,22,27-pentaphenyl- (9CI) (CA INDEX NAME)



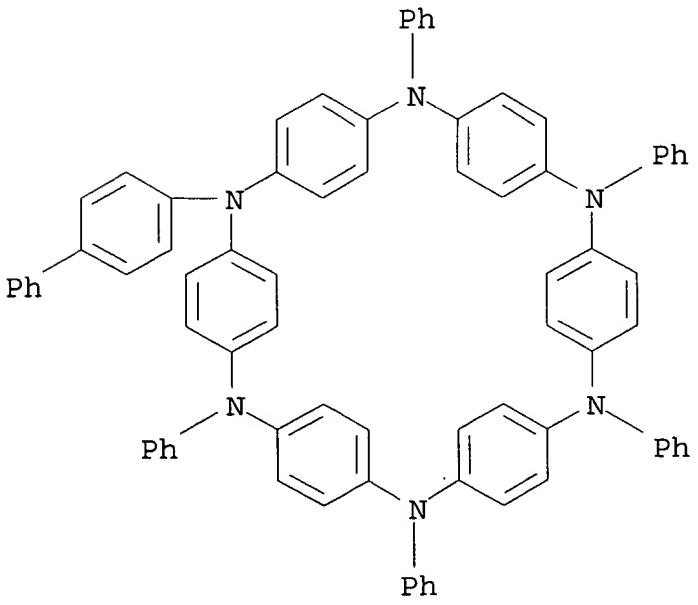
RN 157914-34-6 ZCA

CN 2,7,12,17,22,27-Hexaazaheptacyclo[26.2.2.23,6.28,11.213,16.218,21.223,26]dotetraconta-3,5,8,10,13,15,18,20,23,25,28,30,31,33,35,37,39,41-octadecaene, 2-(4-methoxyphenyl)-7,12,17,22,27-pentaphenyl- (9CI) (CA INDEX NAME)

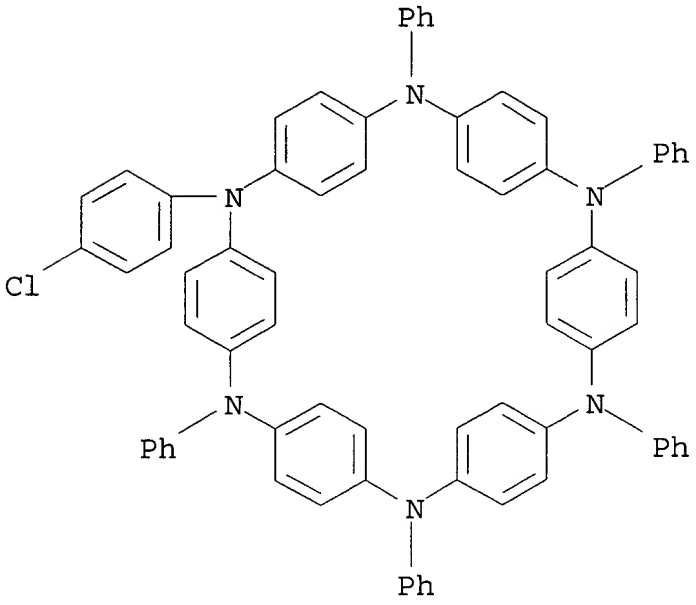


RN 157914-35-7 ZCA

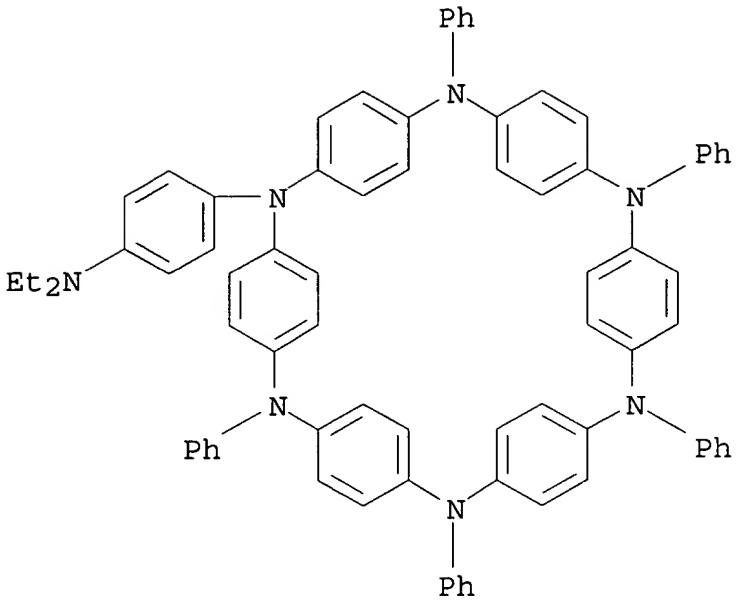
CN 2,7,12,17,22,27-Hexaazaheptacyclo[26.2.2.23,6.28,11.213,16.218,21.223,26]dotetraconta-3,5,8,10,13,15,18,20,23,25,28,30,31,33,35,37,39,41-octadecaene, 2-[1,1'-biphenyl]-4-yl-7,12,17,22,27-pentaphenyl- (9CI) (CA INDEX NAME)



RN 157914-36-8 ZCA
CN 2,7,12,17,22,27-Hexaazaheptacyclo[26.2.2.23,6.28,11.213,16.218,21.223,26]dotetraconta-3,5,8,10,13,15,18,20,23,25,28,30,31,33,35,37,39,41-octadecaene, 2-(4-chlorophenyl)-7,12,17,22,27-pentaphenyl- (9CI) (CA INDEX NAME)



RN 157914-37-9 ZCA
CN Benzenamine, N,N-diethyl-4-(7,12,17,22,27-pentaphenyl-2,7,12,17,22,27-hexaazaheptacyclo[26.2.2.23,6.28,11.213,16.218,21.223,26]dotetraconta-3,5,8,10,13,15,18,20,23,25,28,30,31,33,35,37,39,41-octadecaen-2-yl)- (9CI) (CA INDEX NAME)



RN 157914-38-0 ZCA
CN 2,7,12,17,22,27-Hexaazaheptacyclo[26.2.2.23,6.28,11.213,16.218,21.223,26]dotetraconta-3,5,8,10,13,15,18,20,23,25,28,30,31,33,35,37,39,41-octadecaene, 2,7,17,22-tetrakis(4-methylphenyl)-12,27-diphenyl- (9CI) (CA INDEX NAME)

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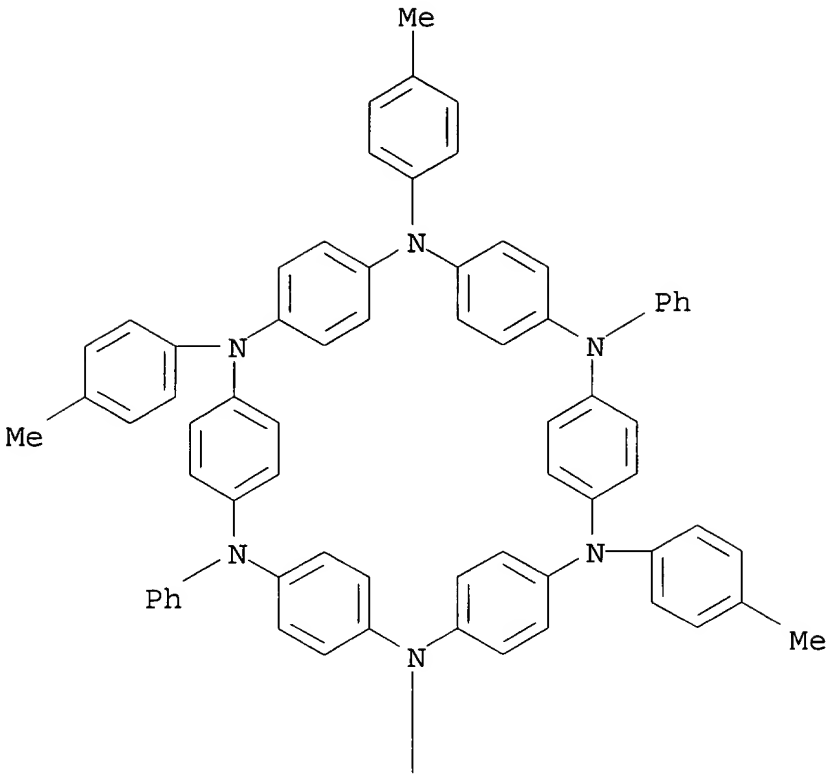

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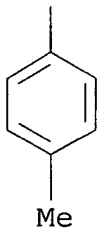

RN 157914-39-1 ZCA
CN 2,7,12,17,22,27-Hexaazaheptacyclo[26.2.2.23,6.28,11.213,16.218,21.223,26]dotetraconta-3,5,8,10,13,15,18,20,23,25,28,30,31,33,35,37,39,41-octadecaene, 2,7,12,17,22-pentakis(4-methylphenyl)-27-phenyl- (9CI) (CA INDEX NAME)

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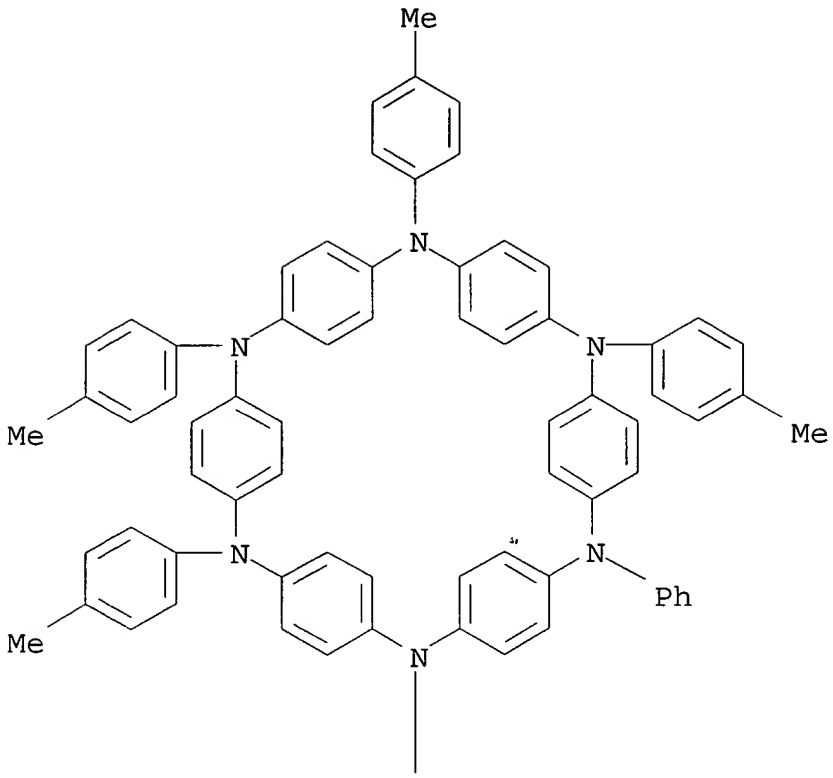

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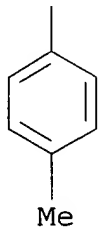
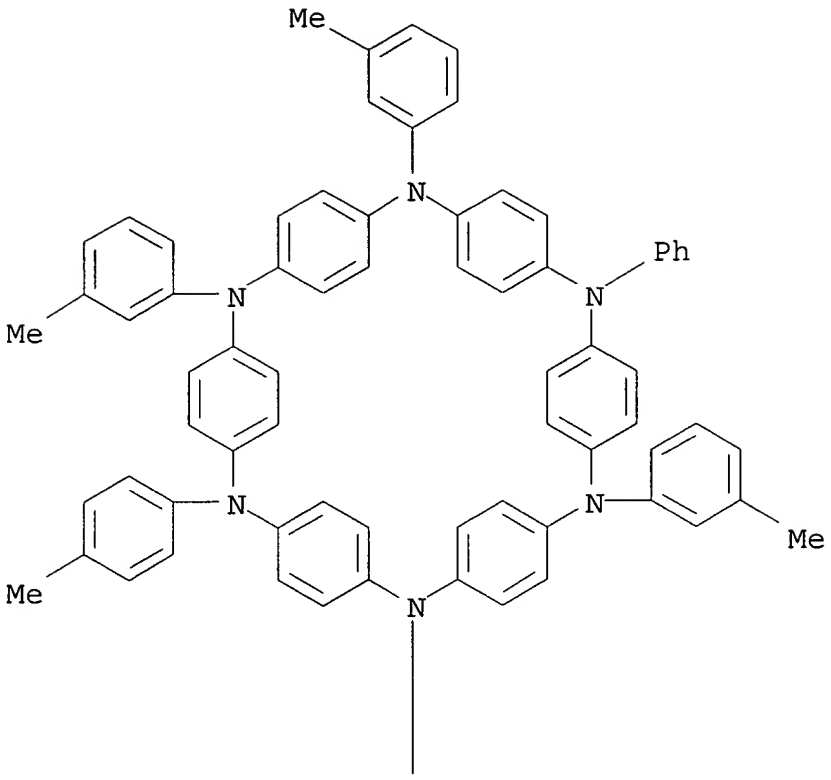


RN 157914-40-4 ZCA
CN 2,7,12,17,22,27-Hexaazaheptacyclo[26.2.2.23,6.28,11.213,16.218,21.223,26]dotetraconta-3,5,8,10,13,15,18,20,23,25,28,30,31,33,35,37,39,41-octadecaene, 2,7,17,22-tetrakis(3-methylphenyl)-12-(4-methylphenyl)-27-phenyl- (9CI) (CA INDEX NAME)

PAGE 1-A



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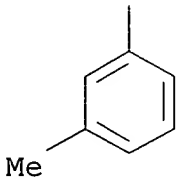


IT **157914-30-2 157914-31-3 157914-32-4**
157914-33-5 157914-34-6 157914-35-7
157914-36-8 157914-37-9 157914-38-0
157914-39-1 157914-40-4
(electrophotog. photoreceptor using)

L13 ANSWER 19 OF 27 ZCA COPYRIGHT 2003 ACS
121:102451 Steroid cyclophanes as artificial receptors embedded in synthetic bilayer membranes: aggregation behavior and molecular recognition. Kikuchi, Junichi; Inada, Masahiko; Miura, Hideaki; Suehiro, Kazuaki; Hayashida, Osamu; Murakami, Yukito (Inst. Fundam.

Res. Org. Chem., Kyushu Univ., Fukuoka, 812, Japan). Recueil des Travaux Chimiques des Pays-Bas, 113(4), 216-21 (English) 1994. CODEN: RTCPA3. ISSN: 0165-0513.

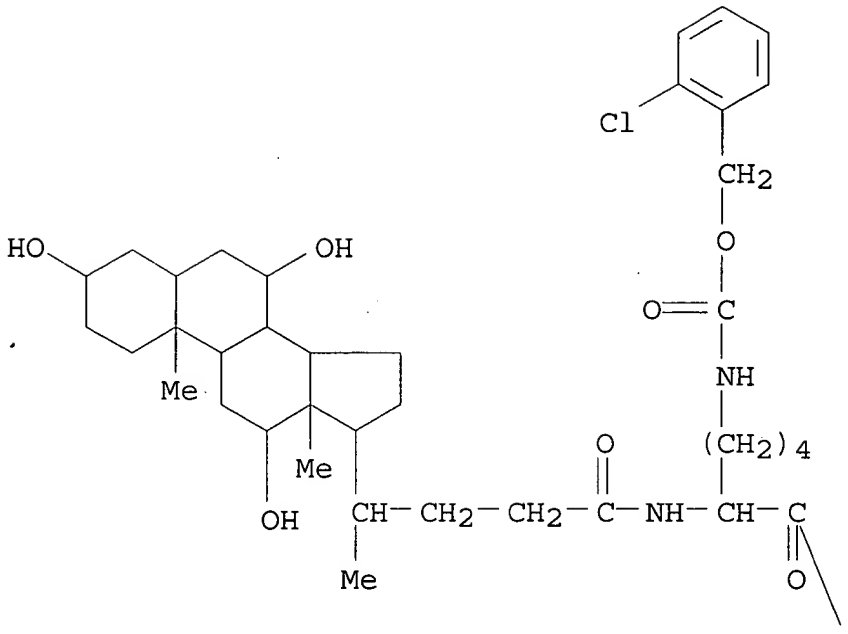
AB Two steroid cyclophanes (I and II), having individually L-lysine and L-aspartate residues as connector units interposed between a 1,6,20,25-tetraaza[6.1.6.1]paracyclophane skeleton and 4 cholate moieties, resp., were designed and synthesized. The cationic steroid cyclophane I, having L-lysine residues, binds anionic and nonionic guests very efficiently, while it has no capacity to bind a guest with a pos. charge in aq. soln. On the other hand, the anionic steroid cyclophane II, bearing L-aspartate residues, shows good binding affinity toward hydrophobic guests in aq. soln. regardless of their charged states. Aggregate morphol. of the cationic and anionic peptide lipids, involving an L-alanine residue interposed between a charged head moiety and a hydrophobic double-chain segment, in the sonicated vesicular state was not perturbed significantly upon formation of hybrid assemblies with the steroid cyclophanes in 2.5 mol%. Even though the anionic bilayer vesicle interacts only weakly with anionic guests, the corresponding hybrid assembly formed with the cationic steroid cyclophane is capable of marked mol. recognition of anionic guests, along with shape-sensitive discrimination, through electrostatic and hydrophobic interactions in aq. soln. In a similar manner, the cationic bilayer membrane alone is incapable of binding a cationic guest. However, the guest-binding ability is not much enhanced in the presence of the anionic steroid cyclophane. Consequently, the cationic steroid cyclophane can act as an efficient cell-surface receptor model for anionic guests while the anionic steroid cyclophane is not a good receptor model when both are embedded in bilayer membranes.

IT **156842-47-6P 156916-65-3P**
(prepn. and hydrogenation of)

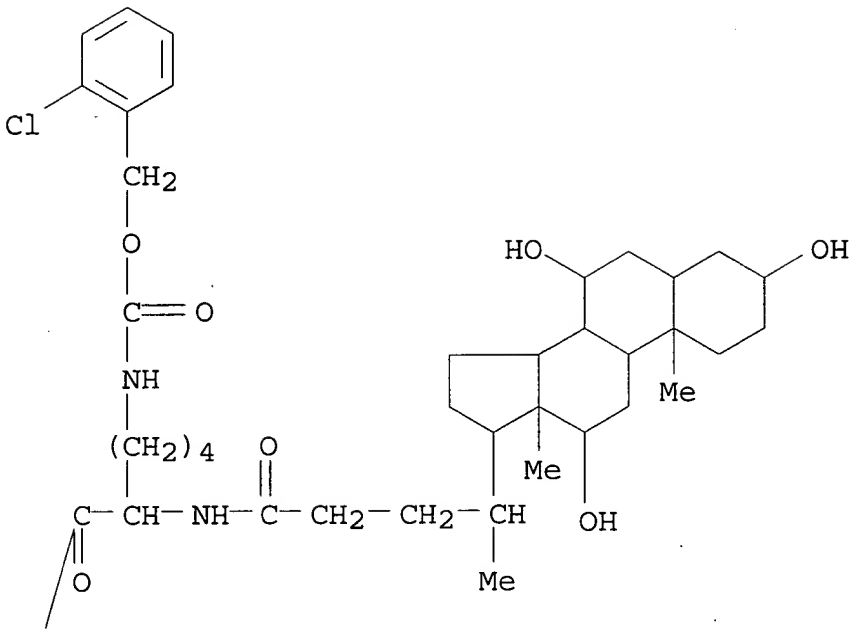
RN 156842-47-6 ZCA

CN Carbamic acid, [7,12,22,27-tetraazapentacyclo[26.2.2.23,6.213,16.218,21]octatriaconta-3,5,13,15,18,20,28,30,31,33,35,37-dodecaene-7,12,22,27-tetrayltetrakis[6-oxo-5-[[[3.alpha.,5.beta.,7.alpha.,12.alpha.,24(S)]-3,7,12-trihydroxy-24-oxocholan-24-yl]amino]-6,1-hexanediyl]]tetrakis-, tetrakis[(2-chlorophenyl)methyl] ester (9CI) (CA INDEX NAME)

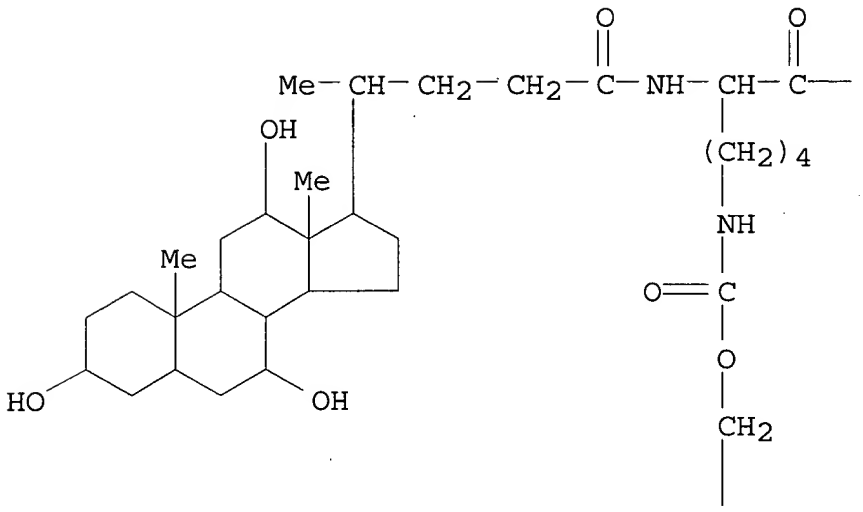
PAGE 1-A



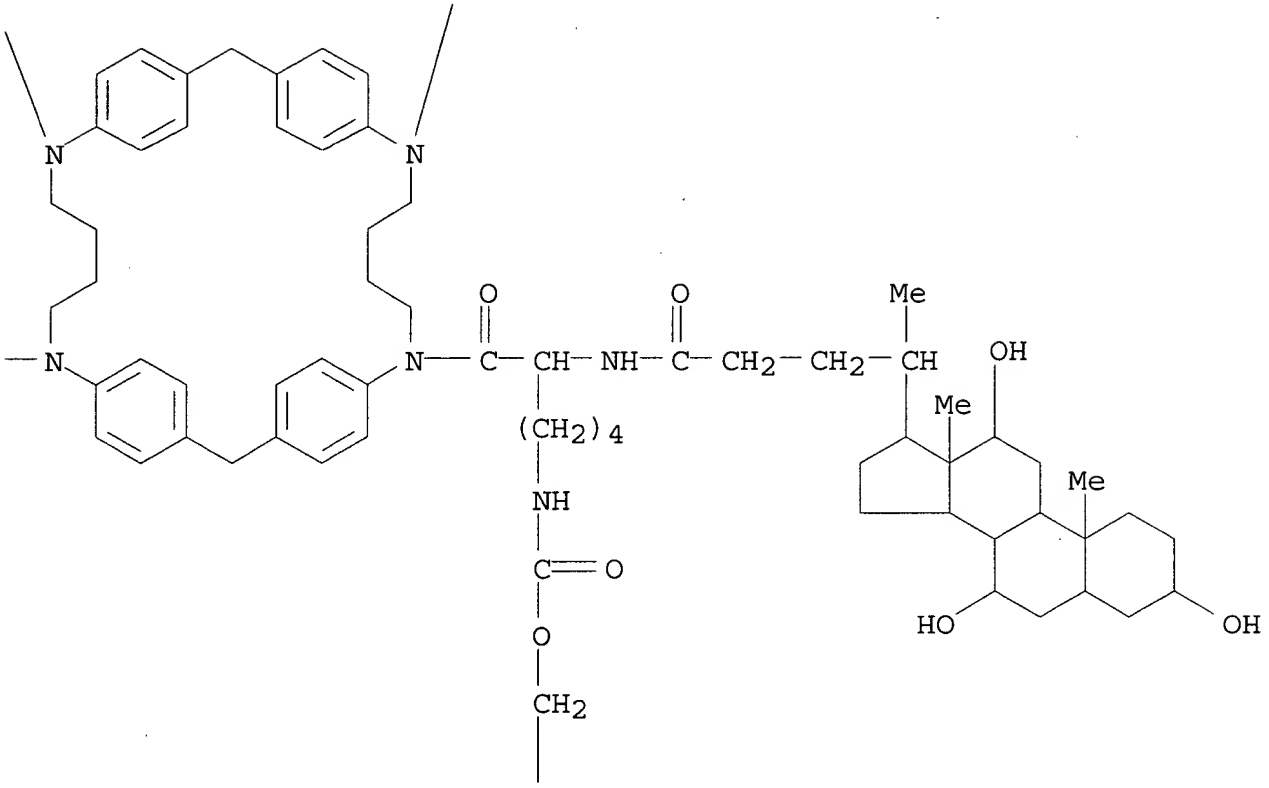
PAGE 1-B



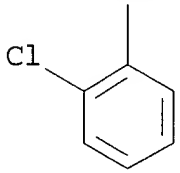
PAGE 2-A



PAGE 2-B



PAGE 3-A



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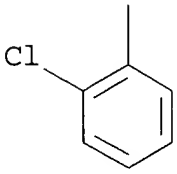
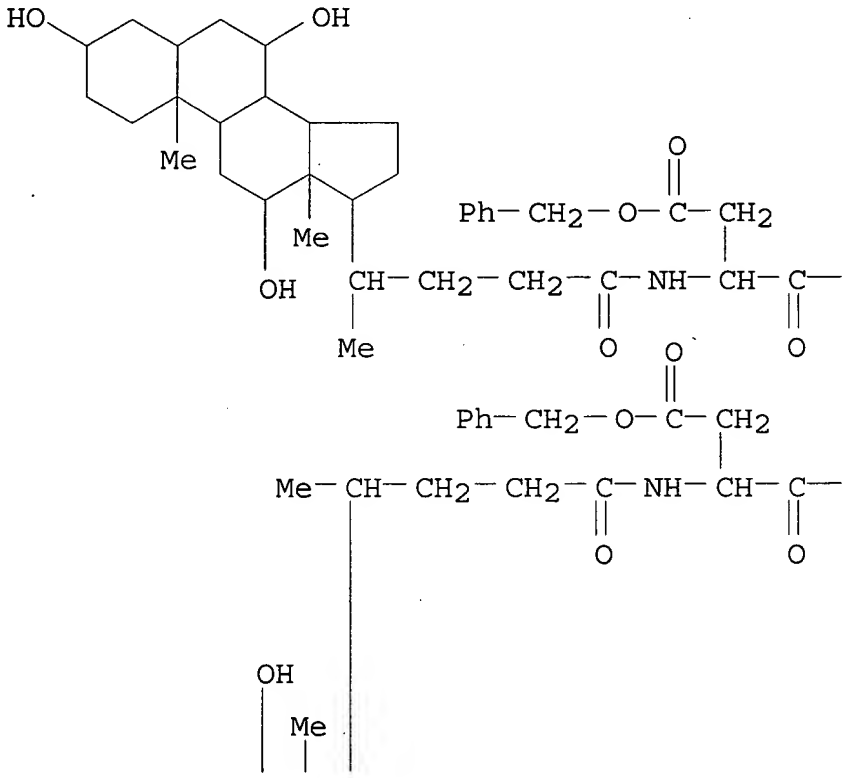


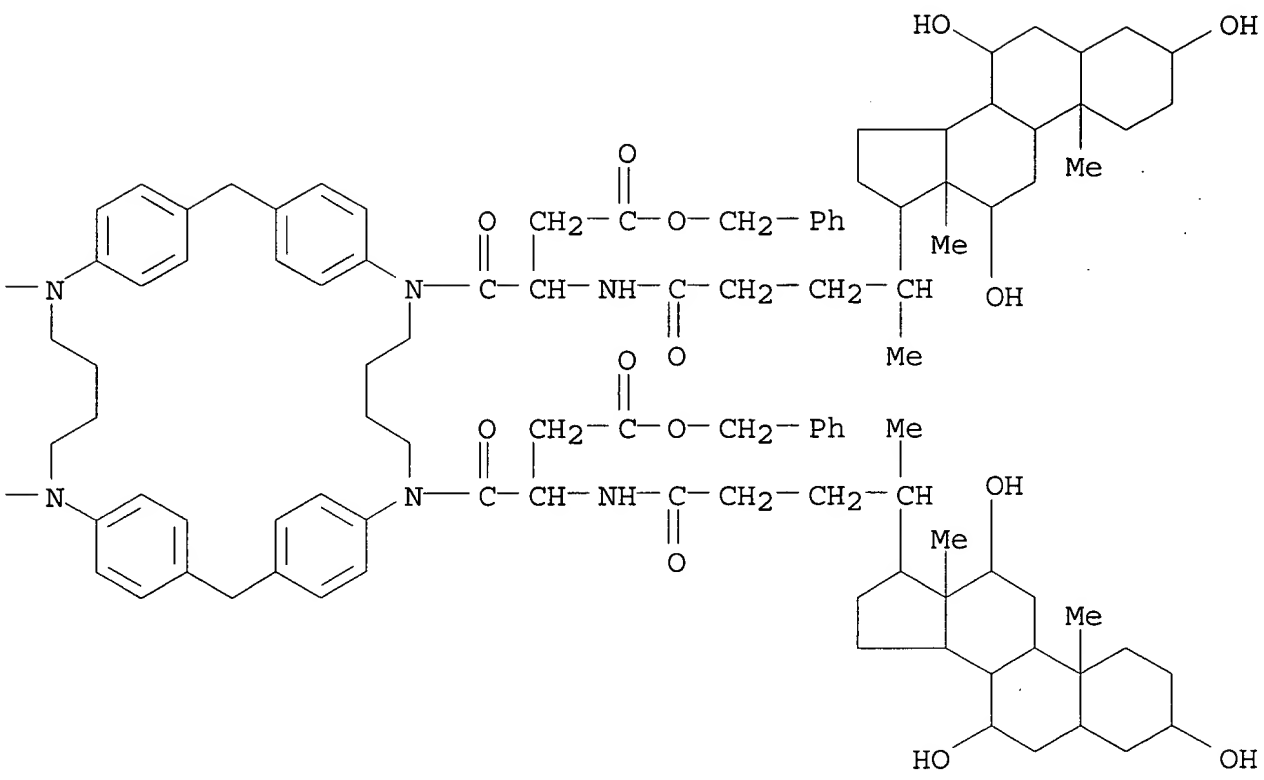
RN 156916-65-3 ZCA

CN 7,12,22,27-Tetraazapentacyclo[26.2.2.23,6.213,16.218,21]octatriacont a-3,5,13,15,18,20,28,30,31,33,35,37-dodecaene-7,12,22,27-tetrabutanoic acid, .gamma.,.gamma.',.gamma.'',.gamma.'''-tetraoxo-.beta.-.beta.',.beta.'',.beta.'''-tetrakis[[(3.alpha.,5.beta.,7.alpha.,12.alpha.)-3,7,12-trihydroxy-24-oxocholan-24-yl]amino]-, tetrakis(phenylmethyl) ester, [.beta.S-(.beta.R*,.beta.'R*,.beta.''R*,.beta.'''R*)]- (9CI) (CA INDEX NAME)

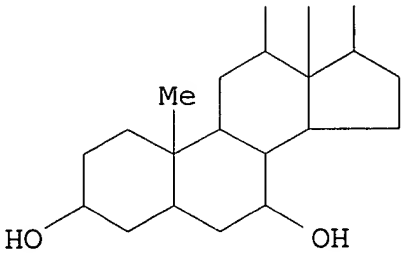
PAGE 1-A



PAGE 1-B



PAGE 2-A



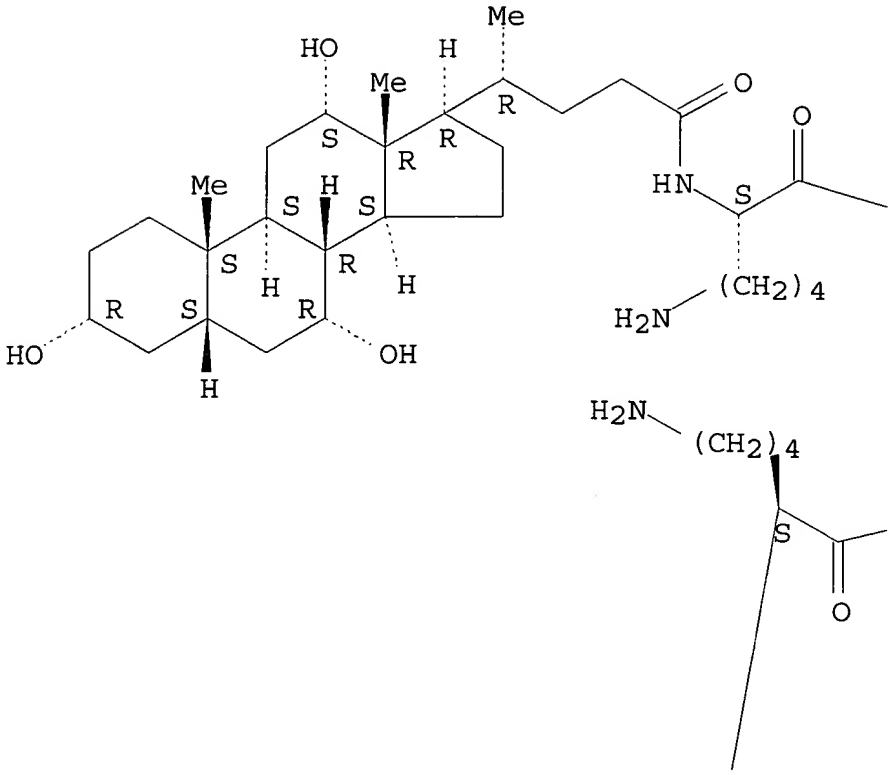
IT **156842-46-5P 156881-79-7P**
(prepn. and mol. recognition properties of, as artificial membrane receptor)

RN 156842-46-5 ZCA

CN Cholan-24-amide, N,N',N'',N'''-[7,12,22,27-tetraazapentacyclo[26.2.2.23,6.213,16.218,21]octatriaconta-3,5,13,15,18,20,28,30,31,33,35,37-dodecaene-7,12,22,27-tetrayltetrakis[1-(4-aminobutyl)-2-oxo-2,1-ethanediyl]]tetrakis[3,7,12-trihydroxy-, tetrahydrochloride, stereoisomer (9CI) (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A



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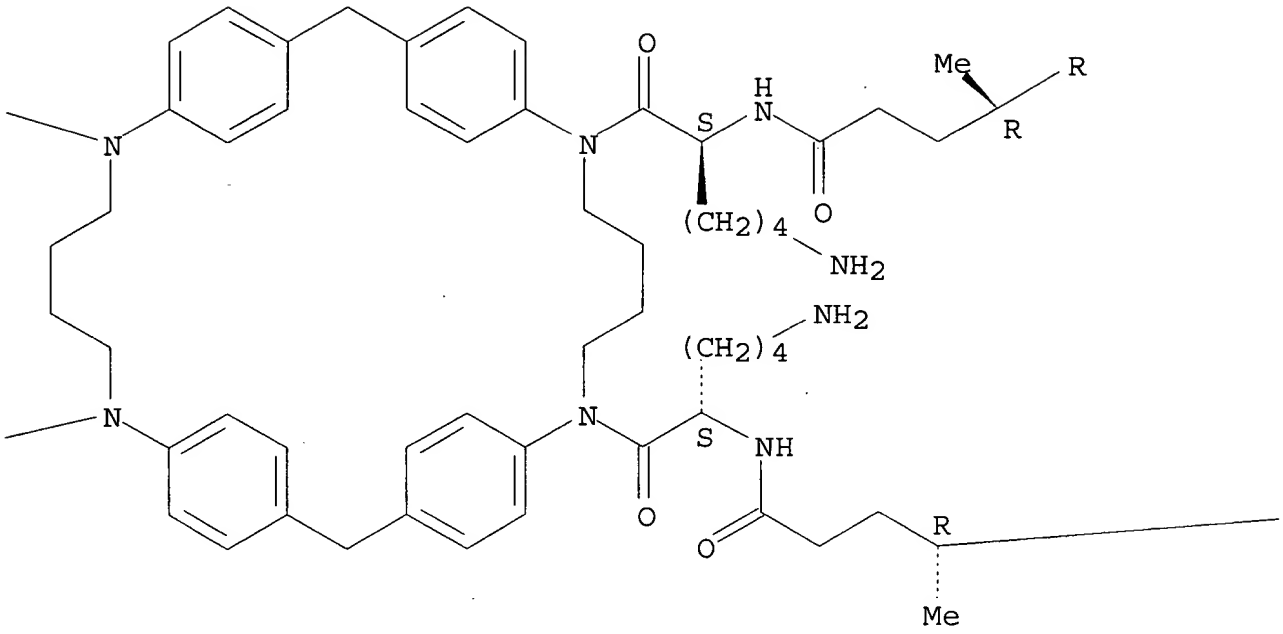

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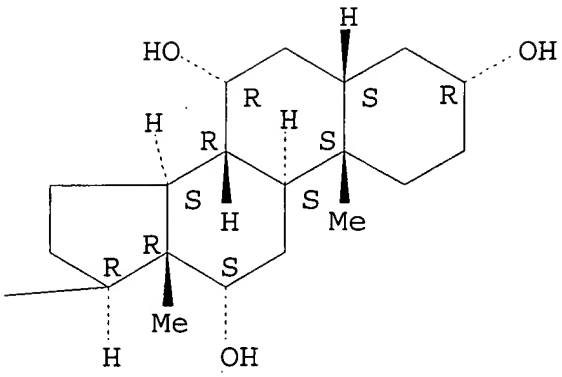

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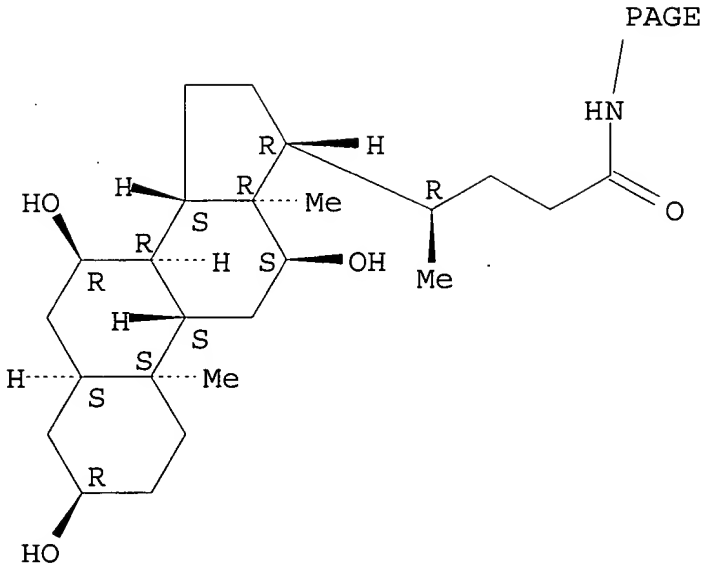
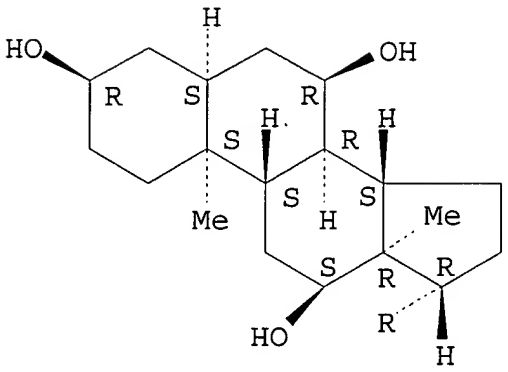


PAGE 3-A

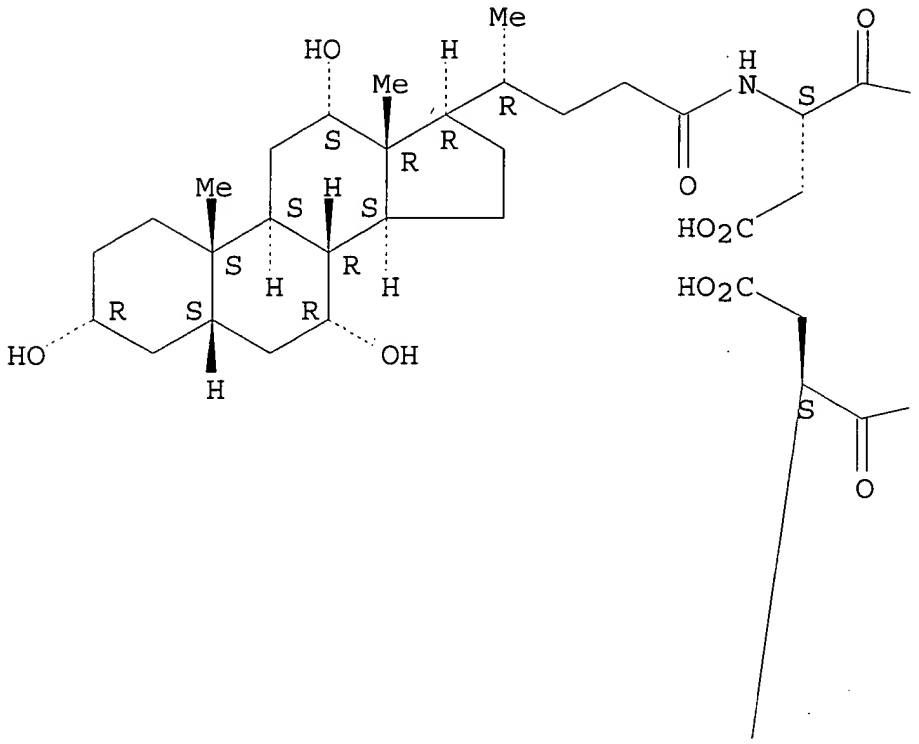


● 4 HCl

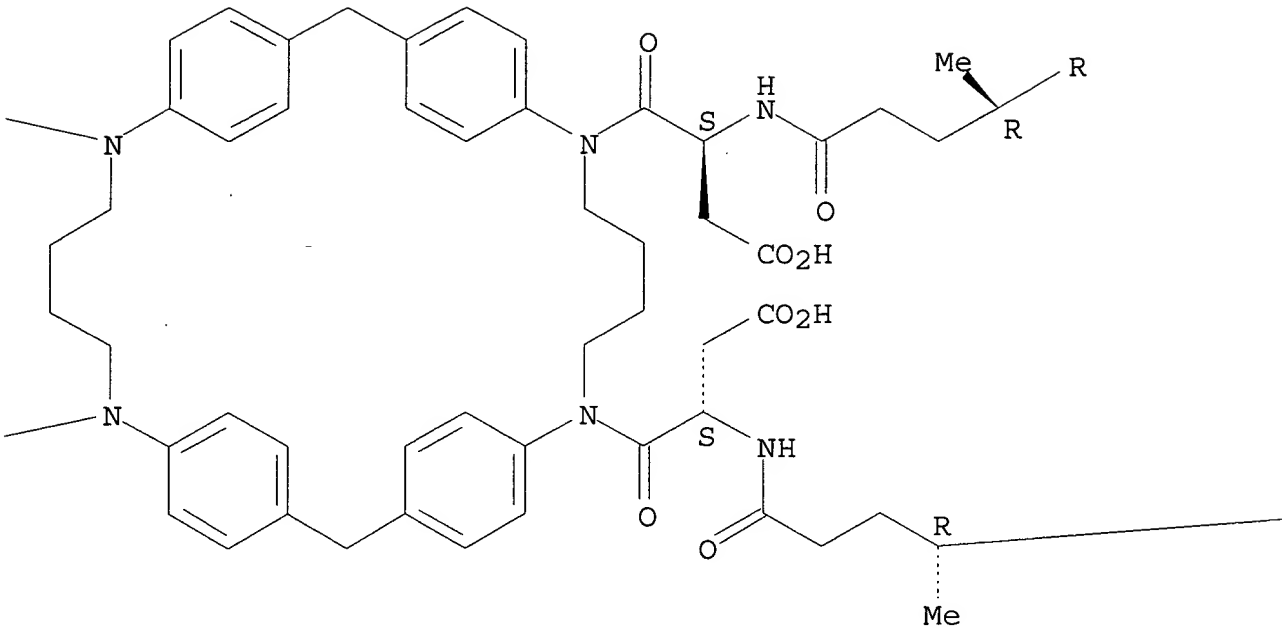
RN 156881-79-7 ZCA
CN 7,12,22,27-Tetraazapentacyclo[26.2.2.23,6.213,16.218,21]octatriacont a-3,5,13,15,18,20,28,30,31,33,35,37-dodecaene-7,12,22,27-tetrabutanoic acid, .gamma.,.gamma.',.gamma.'',.gamma.'''-tetraoxo-.beta.,.beta.',.beta.'',.beta.'''-tetrakis[[(3.alpha.,5.beta.,7.alpha.,12.alpha.)-3,7,12-trihydroxy-24-oxocholan-24-yl]amino]-, (.beta.S,.beta.'S,.beta.''S,.beta.'''S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A



PAGE 1-B



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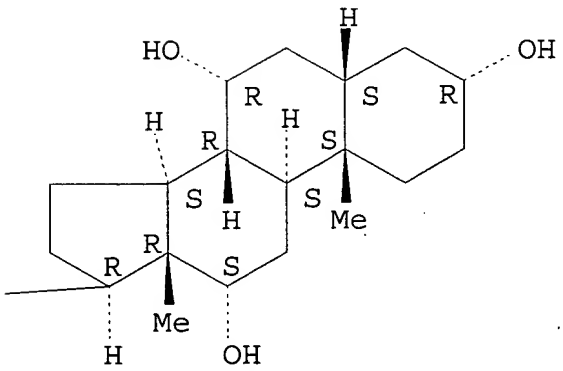

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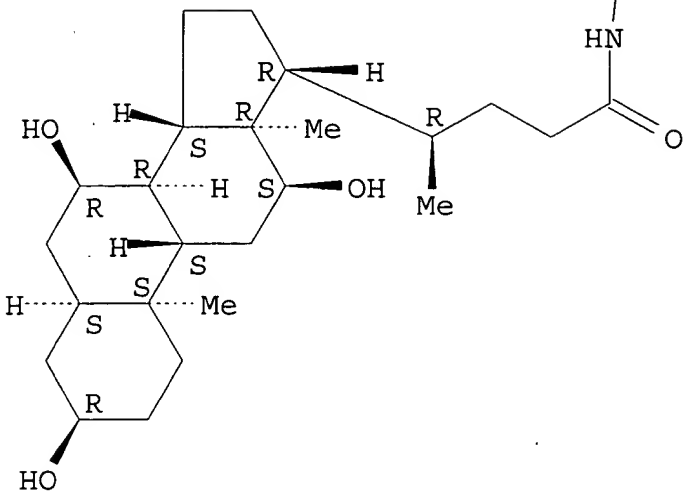
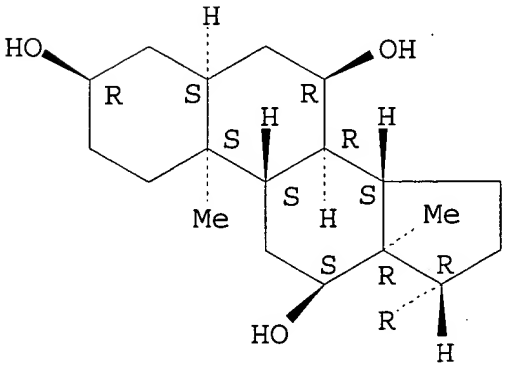
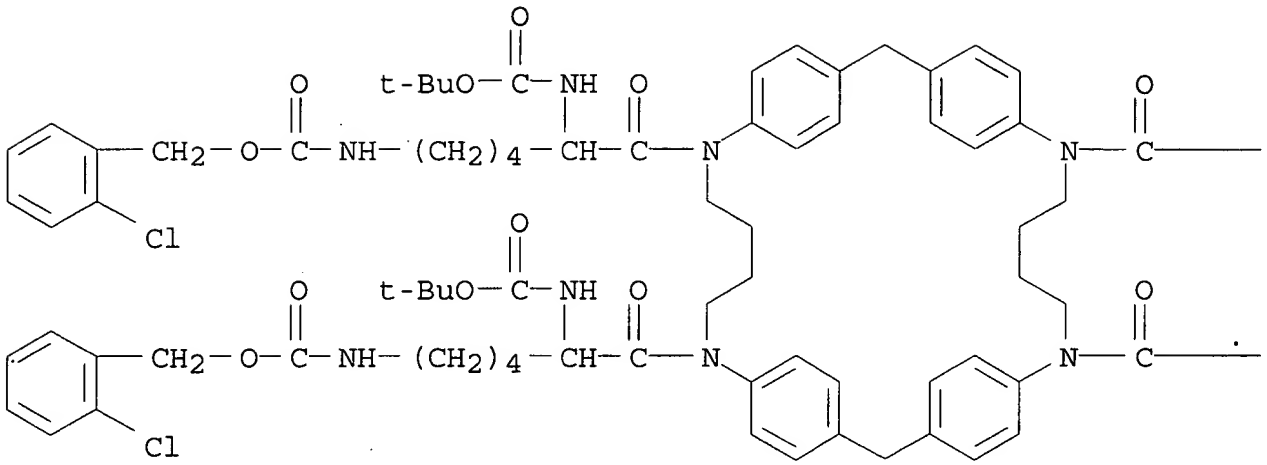


PAGE 3-A



IT **156873-03-9P 156873-04-0P**
(prepn. and reaction with cholic acid)
RN 156873-03-9 ZCA
CN Carbamic acid, [7,12,22,27-tetraazapentacyclo[26.2.2.23,6.213,16.218,21]octatriaconta-3,5,13,15,18,20,28,30,31,33,35,37-dodecaene-7,12,22,27-tetrayltetrakis[1-[4-[[[(2-chlorophenyl)methoxy]carbonyl]amino]butyl]-2-oxo-2,1-ethanediyl]]tetrakis-, tetrakis(1,1-dimethylethyl) ester (9CI) (CA INDEX NAME)

PAGE 1-A



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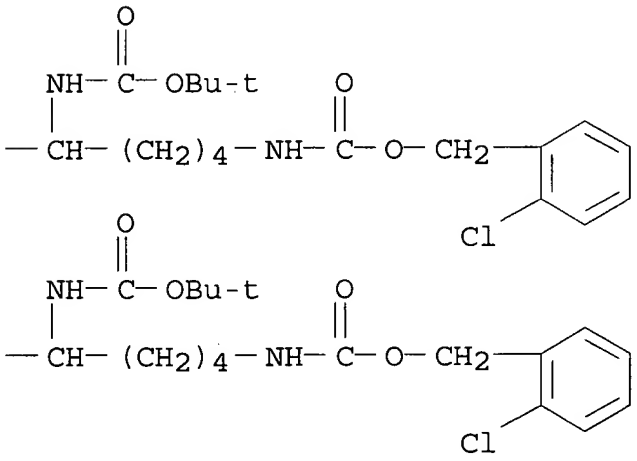
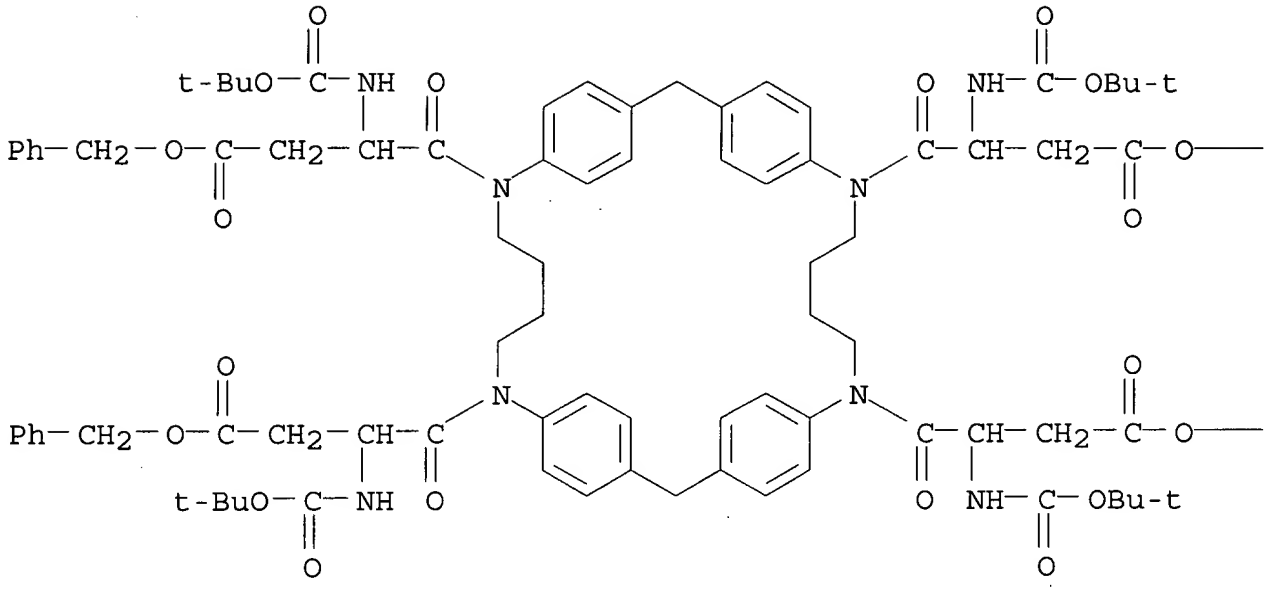


RN 156873-04-0 ZCA
CN 7,12,22,27-Tetraazapentacyclo[26.2.2.23,6.213,16.218,21]octatriaconta-3,5,13,15,18,20,28,30,31,33,35,37-dodecaene-7,12,22,27-tetrabutanoic acid, .beta.,.beta.',.beta.'',.beta.'''-tetrakis[[(1,1-dimethylethoxy)carbonyl]amino]-.gamma.,.gamma.',.gamma.'',.gamma.'''-tetraoxo-, tetrakis(phenylmethyl) ester (9CI) (CA INDEX NAME)

PAGE 1-A



PAGE 1-B

— CH_2 — Ph

— CH_2 — Ph

IT **156842-47-6P 156916-65-3P**
(prepn. and hydrogenation of)
IT **156842-46-5P 156881-79-7P**
(prepn. and mol. recognition properties of, as artificial membrane receptor)
IT **156873-03-9P 156873-04-0P**
(prepn. and reaction with cholic acid)

L13 ANSWER 20 OF 27 ZCA COPYRIGHT 2003 ACS
116:255595 Synthesis of bicyclic bis-intercaland derivatives of acridine. Claude, Sylvain; Lehn, Jean Marie; Perez de Vega, Maria Jesus; Vigneron, Jean Pierre (Lab. Chim. Interact. Mol., Coll. France, Paris, 75005, Fr.). New Journal of Chemistry, 16(1-2), 21-8 (French) 1992. CODEN: NJCHE5. ISSN: 0398-9836.
GI

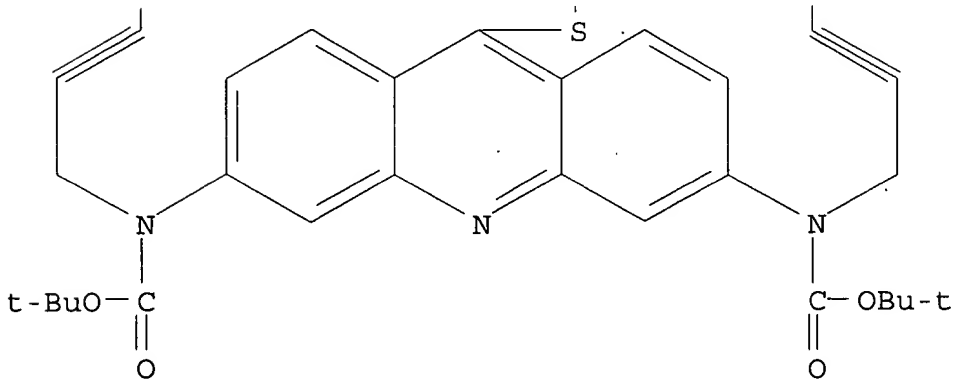
* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

AB Title compds. I [X = O, X1 = (CH2)6, (CH2CH2O)nCH2CH2, n = 1, 2; X = NCO2CMe3, X1 = CH2CH2OCH2CH2, CH2X2CH2, X2 = 2,6-pyridinediyl] were prepd. via intramol. cyclization of the alkynes II with Cu(OAc)2. I were quaternized, making them water-sol.
IT **141468-51-1P 141468-52-2P**
(prepn. and quaternization of)
RN 141468-51-1 ZCA
CN 3,24-(Imino[2,4]hexadiynimino)-6,19:18,21-dimetheno[1,4,23,10,17]oxadithiadiazacyclopentacosino[6,5-c:21,22-c']diquinoline-10,17,34,41-tetracarboxylic acid, 12,13,14,15-tetradehydro-11,16,28,29,31,32-hexahydro-, tetrakis(1,1-dimethylethyl) ester (9CI) (CA INDEX NAME)

PAGE 1-A

PAGE 2-A

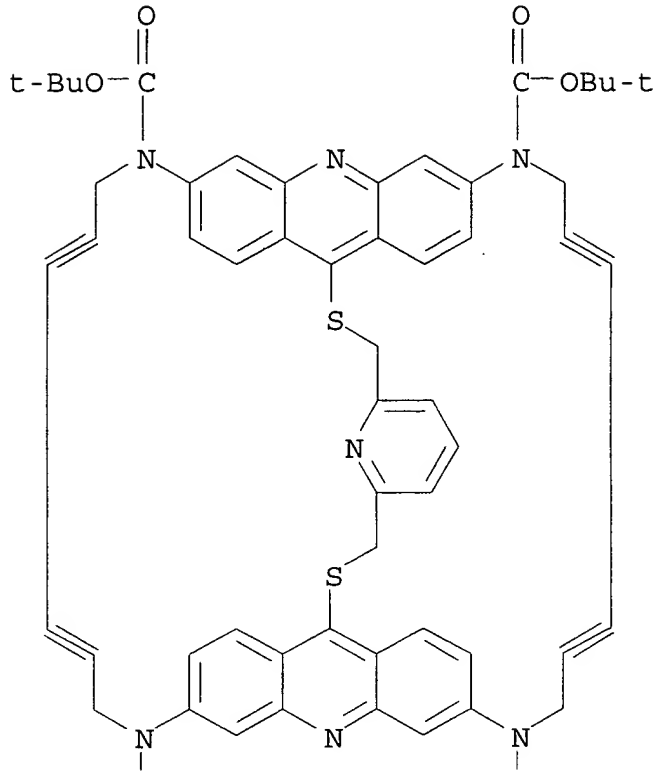
PAGE 3-A



RN 141468-52-2 ZCA
CN 34H-3,24-(Imino[2,4]hexadiynimino)-6,9:18,21-dimetheno-29,33-nitrilo-28H-[1,20,7,14]dithiadiazacycloheptacosino[3,2-c:18,19-c']diquinoline-10,17,37,44-tetracarboxylic acid, 12,13,14,15-tetradehydro-11,16-dihydro-, tetrakis(1,1-dimethylethyl)

ester (9CI) (CA INDEX NAME)

PAGE 1-A



PAGE 2-A

IT **141468-51-1P 141468-52-2P**
(prepn. and quaternization of)

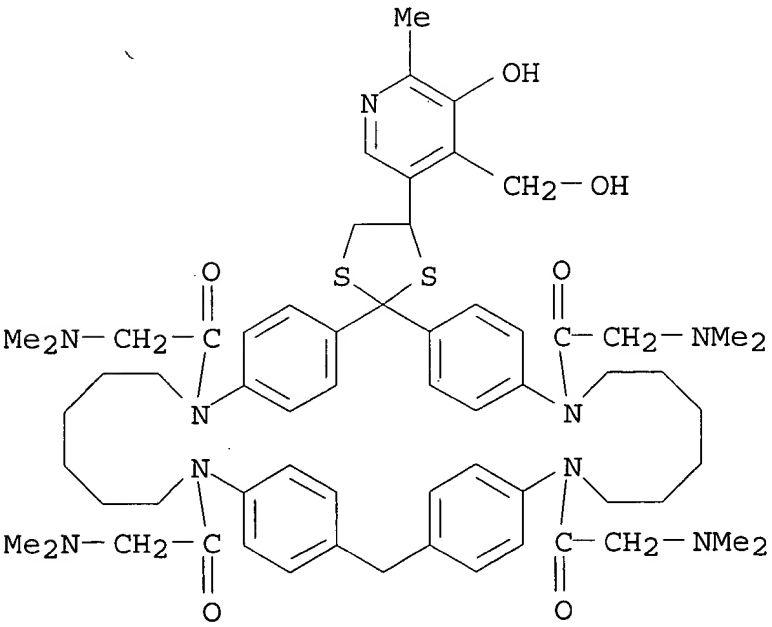
L13 ANSWER 21 OF 27 ZCA COPYRIGHT 2003 ACS
113:36983 Artificial transaminases linking pyridoxamine to binding cavities: controlling the geometry. Breslow, Ronald; Canary, James W.; Varney, Michael; Waddell, Sherman T.; Yang, Dan (Dep. Chem., Columbia Univ., New York, NY, 10027, USA). Journal of the American Chemical Society, 112(13), 5212-19 (English) 1990. CODEN: JACSAT. ISSN: 0002-7863. OTHER SOURCES: CASREACT 113:36983.
AB A transaminase mimic joining a pyridoxamine unit to a cyclodextrin

by a single kinase is quite selective for the conversion of phenylpyruvic acid to phenylalanine, compared with its reactivity toward nonbinding keto acids. The selectivity is even greater with 4-tert-butylphenylpyruvic acid but is essentially erased with a phenylpyruvic acid carrying a tert-Bu group in the meta position. This strong geometric preference can be modified with transaminase mimics in which the pyridoxamine is joined to cyclodextrin by 2 links, greatly restricting the freedom of the system. A transaminase has also been prepd. with the pyridoxamine unit doubly linked to a synthetic macrocyclic hydrophobic cavity, which has yet other geometric preferences. The doubly linked pyridoxamine units were prepd. by use of a novel synthetic procedure for the conversion of olefins in vic-dithiols. An improved procedure for the prepn. of .beta.-cyclodextrin 6A,6B diiodide is also described.

IT **127516-87-4P**
(prepn. and conversion to (dimethylamino)amide pyridoxalimine)

RN 127516-87-4 ZCA

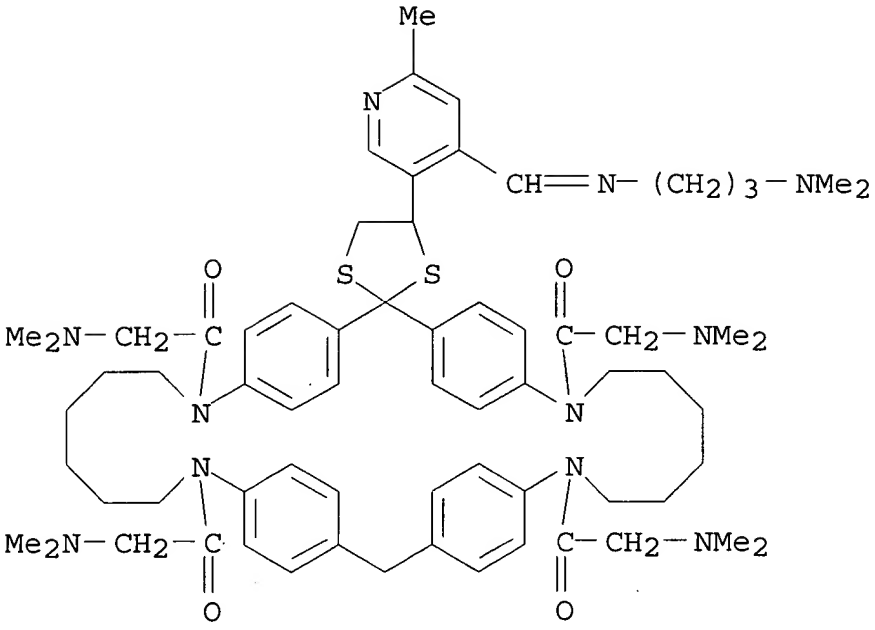
CN Spiro[1,3-dithiolane-2,2'-[7,14,24,31]tetraazapentacyclo[30.2.2.23,6.215,18.220,23]dotetraconta[3,5,15,17,20,22,32,34,35,37,39,41]dodecaene], 7',14',24',31'-tetrakis[(dimethylamino)acetyl]-4-[5-hydroxy-4-(hydroxymethyl)-6-methyl-3-pyridinyl]- (9CI) (CA INDEX NAME)



IT **127516-88-5P**
(prepn. and conversion to (dimethylamino)amide pyridoxamine)

RN 127516-88-5 ZCA

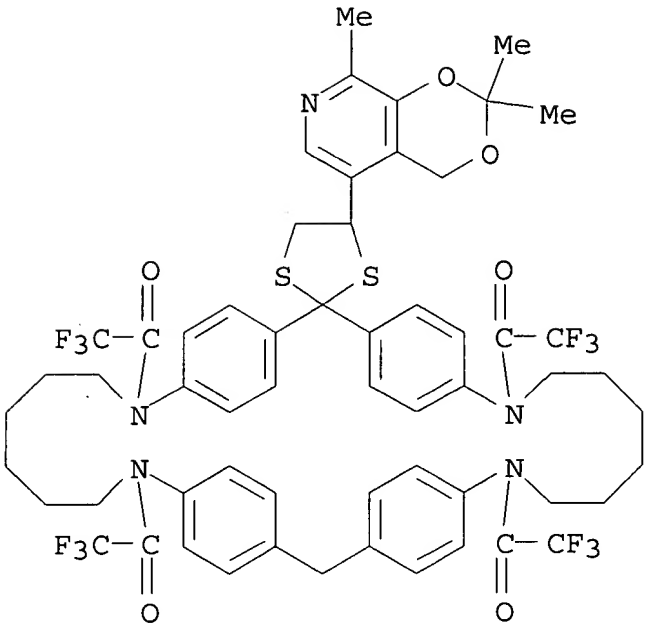
CN Spiro[1,3-dithiolane-2,2'-[7,14,24,31]tetraazapentacyclo[30.2.2.23,6.215,18.220,23]dotetraconta[3,5,15,17,20,22,32,34,35,37,39,41]dodecaene], 7',14',24',31'-tetrakis[(dimethylamino)acetyl]-4-[4-[[[3-(dimethylamino)propyl]imino]methyl]-6-methyl-3-pyridinyl]- (9CI) (CA INDEX NAME)



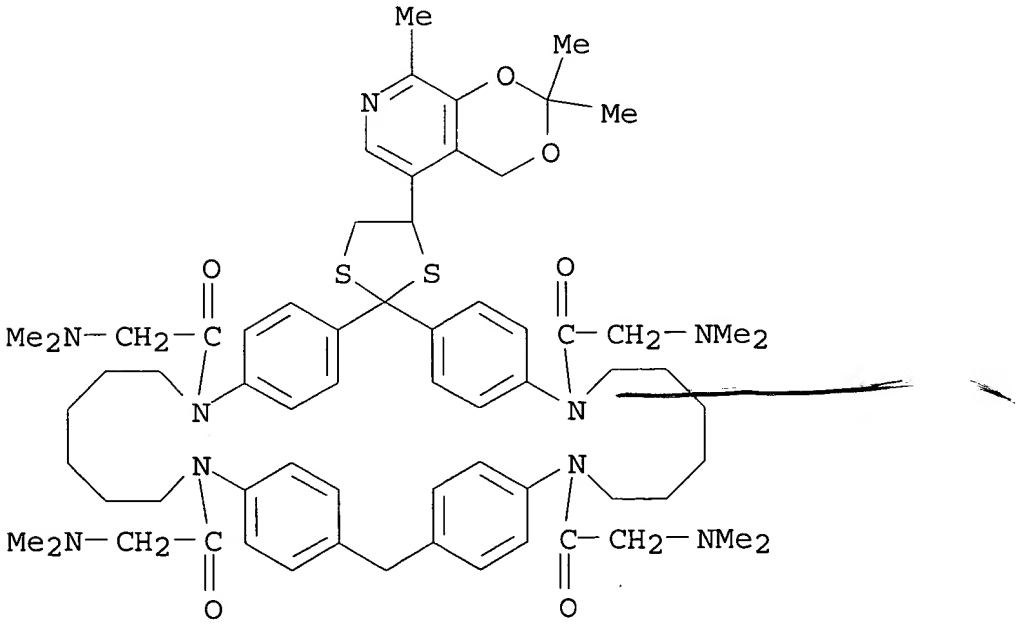
IT **127491-61-6P**
(prepn. and conversion to (dimethylamino)amide pyridoxine acetamide)

RN 127491-61-6 ZCA

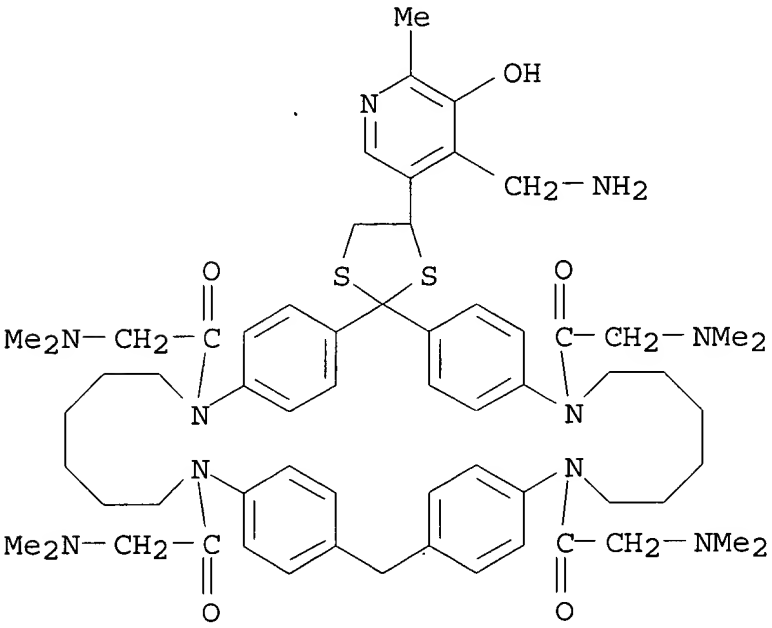
CN Spiro[1,3-dithiolane-2,2'-[7,14,24,31]tetraazapentacyclo[30.2.2.23,6.215,18.220,23]dotetraconta[3,5,15,17,20,22,32,34,35,37,39,41]dodecaene], 7',14',24',31'-tetrakis(trifluoroacetyl)-4-(2,2,8-trimethyl-4H-1,3-dioxino[4,5-c]pyridin-5-yl)- (9CI) (CA INDEX NAME)



IT **127491-62-7P**
(prepn. and conversion to (dimethylamino)amide pyridoxine diol)
RN 127491-62-7 ZCA
CN Spiro[1,3-dithiolane-2,2'-[7,14,24,31]tetraazapentacyclo[30.2.2.23,6.215,18.220,23]dotetraconta[3,5,15,17,20,22,32,34,35,37,39,41]dodecaene], 7',14',24',31'-tetrakis[(dimethylamino)acetyl]-4-(2,2,8-trimethyl-4H-1,3-dioxino[4,5-c]pyridin-5-yl)- (9CI) (CA INDEX NAME)

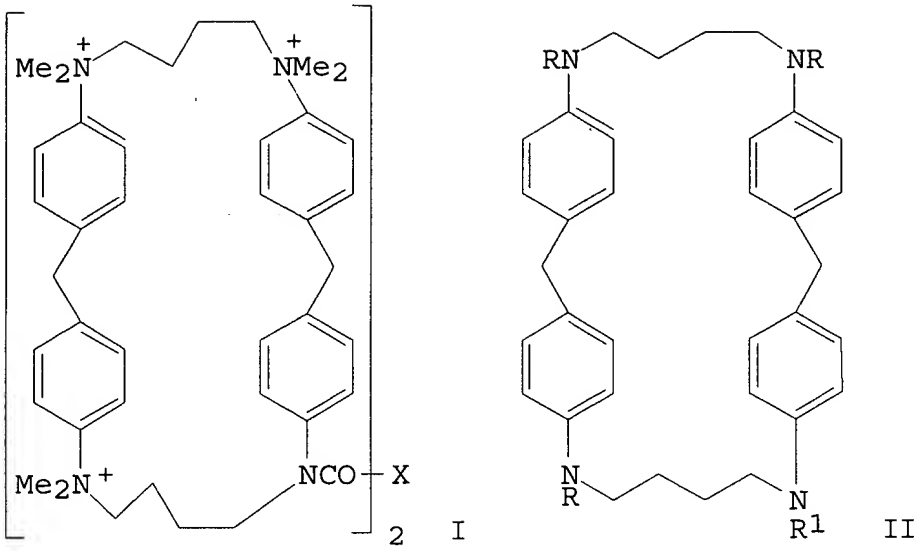


IT **127491-58-1P**
(prepn. and use of artificial transaminase with ketal acids)
RN 127491-58-1 ZCA
CN Spiro[1,3-dithiolane-2,2'-[7,14,24,31]tetraazapentacyclo[30.2.2.23,6.215,18.220,23]dotetraconta[3,5,15,17,20,22,32,34,35,37,39,41]dodecaene], 4-[4-(aminomethyl)-5-hydroxy-6-methyl-3-pyridinyl]-7',14',24',31'-tetrakis[(dimethylamino)acetyl]- (9CI) (CA INDEX NAME)



IT **127516-87-4P**
(prepn. and conversion to (dimethylamino)amide pyridoxalimine)
IT **127516-88-5P**
(prepn. and conversion to (dimethylamino)amide pyridoxamine)
IT **127491-61-6P**
(prepn. and conversion to (dimethylamino)amide pyridoxine acetamide)
IT **127491-62-7P**
(prepn. and conversion to (dimethylamino)amide pyridoxine diol)
IT **127491-58-1P**
(prepn. and use of artificial transaminase with ketal acids)

L13 ANSWER 22 OF 27 ZCA COPYRIGHT 2003 ACS
112:216893 Biomimetic studies using artificial systems. V. Design and synthesis of novel water-soluble bis(cyclophanes). Lai, Chung Fang; Odashima, Kazunori; Koga, Kenji (Fac. Pharm. Sci., Univ. Tokyo, Tokyo, 113, Japan). Chemical & Pharmaceutical Bulletin, 37(9), 2351-4 (English) 1989. CODEN: CPBTAL. ISSN: 0009-2363. OTHER SOURCES: CASREACT 112:216893.
GI



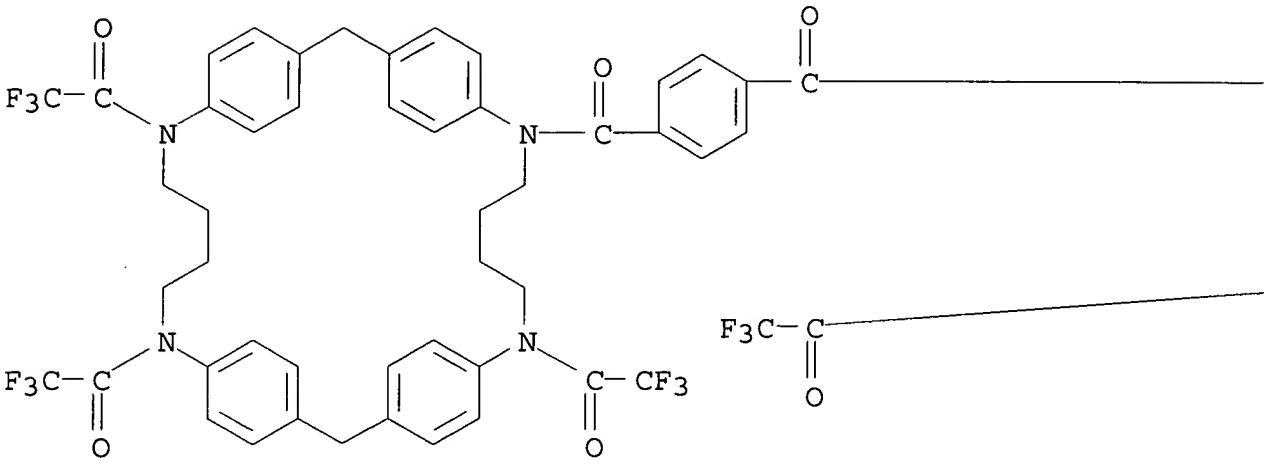
AB Novel water-sol. quaternized aryloylbis(cyclophanes) or alkanoylbis(cyclophanes) I [X = (CH2)3, 1,3-C6H4, 1,4-C6H4], composed of 2 units of paracyclophane II (R = R1 = H) connected by bridges, were prepd. as hosts having 2 discrete hydrophobic cavities to bind 2 guest mols. simultaneously or a single guest mol. via double recognition in neutral water. Glutaryl, terephthaloyl and isophthaloyl groups were used as spacers to bridge the 2 cyclophane units. The bridge formation was carried out using II (R = COCF3, R1 = H) as an intermediate. The details of the synthesis and characterization of duplex hosts I are described.

IT **127136-82-7P 127136-84-9P 127136-86-1P**
(prepn. and hydrolysis of)

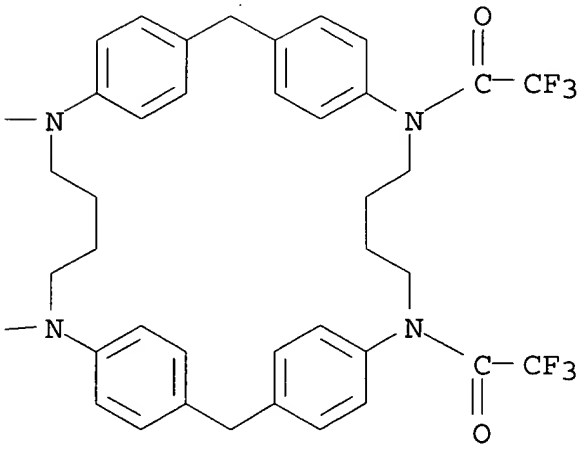
RN 127136-82-7 ZCA

CN 7,12,22,27-Tetraazapentacyclo[26.2.2.23,6.213,16.218,21]octatriaconta-3,5,13,15,18,20,28,30,31,33,35,37-dodecaene, 7,7'-(1,4-phenylenedicarbonyl)bis[12,22,27-tris(trifluoroacetyl)- (9CI) (CA INDEX NAME)

PAGE 1-A

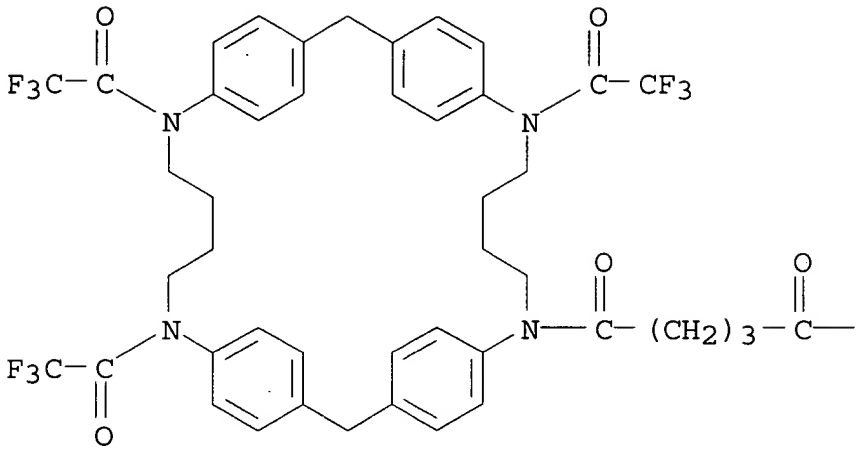


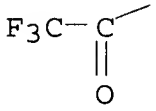
PAGE 1-B



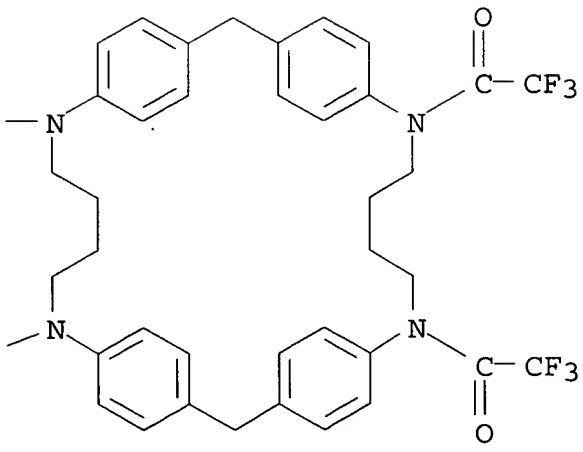
RN 127136-84-9 ZCA
CN 7,12,22,27-Tetraazapentacyclo[26.2.2.23,6.213,16.218,21]octatriaconta-3,5,13,15,18,20,28,30,31,33,35,37-dodecaene, 7,7'-(1,5-dioxo-1,5-pentanediyl)bis[12,22,27-tris(trifluoroacetyl)- (9CI) (CA INDEX NAME)

PAGE 1-A



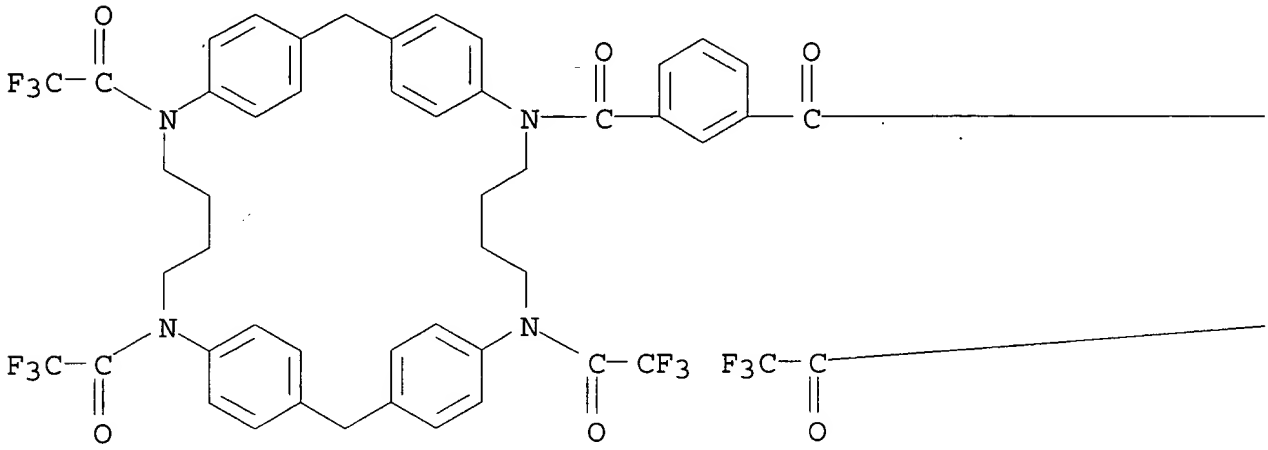


PAGE 1-B

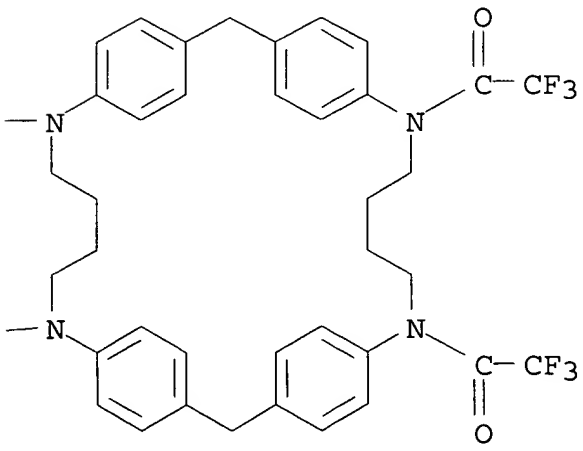


RN 127136-86-1 ZCA
CN 7,12,22,27-Tetraazapentacyclo[26.2.2.23,6.213,16.218,21]octatriacont a-3,5,13,15,18,20,28,30,31,33,35,37-dodecaene, 7,7'-(1,3-phenylenedicarbonyl)bis[12,22,27-tris(trifluoroacetyl)- (9CI) (CA INDEX NAME)

PAGE 1-A



PAGE 1-B

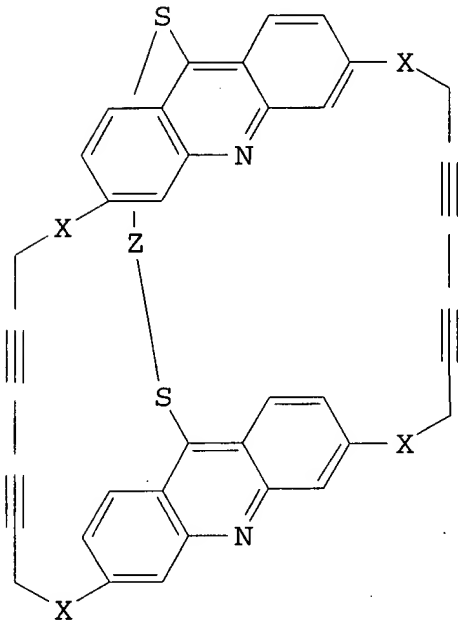


IT **127136-82-7P 127136-84-9P 127136-86-1P**
(prepn. and hydrolysis of)

L13 ANSWER 23 OF 27 ZCA COPYRIGHT 2003 ACS
111:97200 Bicyclo-bis-intercalands: synthesis of triply bridged bis-intercalands based on acridine subunits. Claude, Sylvain; Lehn,

Jean Marie; Vigneron, Jean Pierre (Lab. Chim. Interact. Mol., Coll. France, Paris, 75005, Fr.). Tetrahedron Letters, 30(8), 941-4 (English) 1989. CODEN: TELEAY. ISSN: 0040-4039. OTHER SOURCES: CASREACT 111:97200.

GI



I

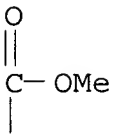
AB Macrobicyclic receptor mols. I [X = O, Z = (CH2)6, CH2CH2OCH2CH2, CH2(CH2OCH2)2CH2; X = NCO2Me, Z = (CH2)6], built on two tripoly-bridged acridine intercalating suubunits, have been synthesized via an efficient procedure involving two intramol. acetylene coupling reactions. Some physicochem. properties of these compds. are reported.

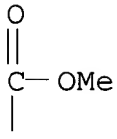
IT **122106-11-0P**
(prepn. and NMR of)

RN 122106-11-0 ZCA

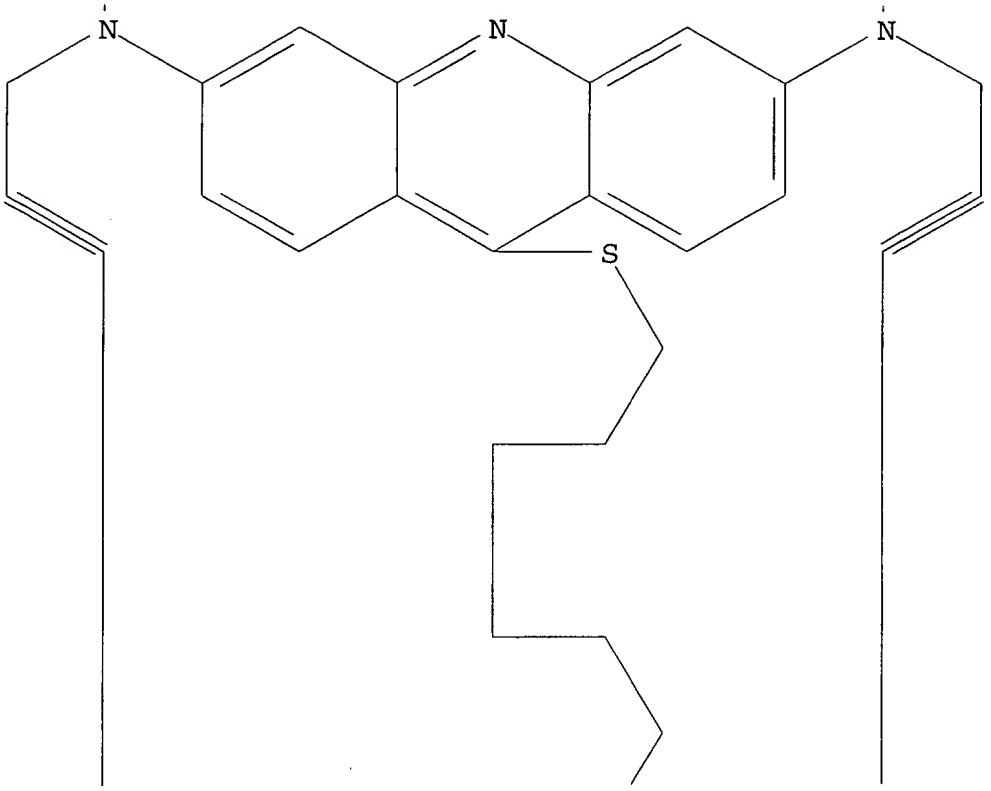
CN 3,24-(Imino[2,4]hexadiynimino)-6,9:18,21-dimetheno[1,20,7,14]dithiadiazacyclohexacosino[3,2-c:18,19-c']diquinoline-10,17,35,42-tetracarboxylic acid, 12,13,14,15-tetradehydro-11,16,28,29,30,31,32,33-octahydro-, tetramethyl ester (9CI) (CA INDEX NAME)

PAGE 1-A

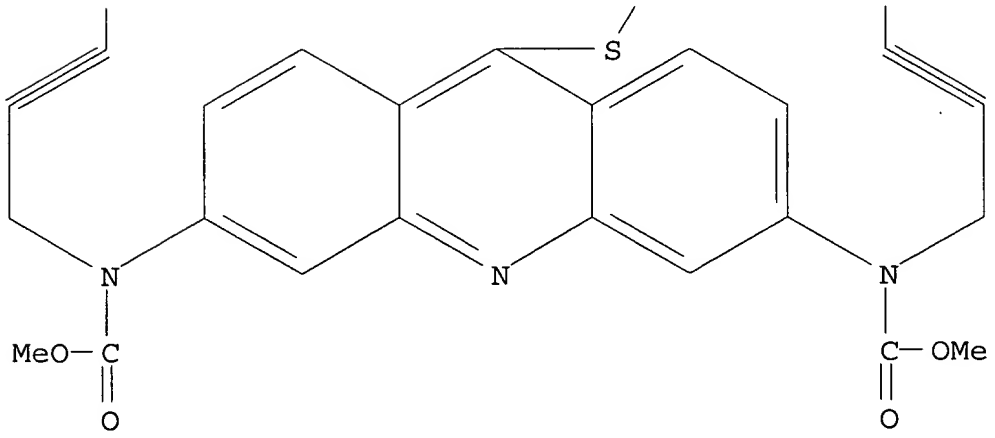




PAGE 2-A

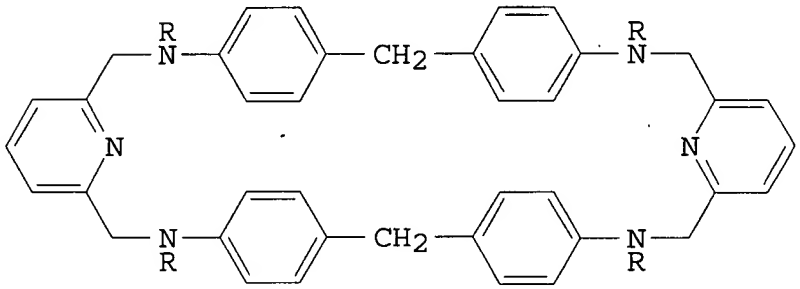


PAGE 3-A



IT **122106-11-0P**
(prepn. and NMR of)

L13 ANSWER 24 OF 27 ZCA COPYRIGHT 2003 ACS
110:95186 A water soluble multisite receptor: synthesis, copper(II) and organic molecule complexation. Fornasier, Roberto; Reniero, Fabiano; Scrimin, Paolo; Tonellato, Umberto (Cent. Mec. Reaz. Org., Univ. Padova, Padua, 35131, Italy). Journal of Inclusion Phenomena, 6(2), 175-81 (English) 1988. CODEN: JOIPDF. ISSN: 0167-7861.
GI



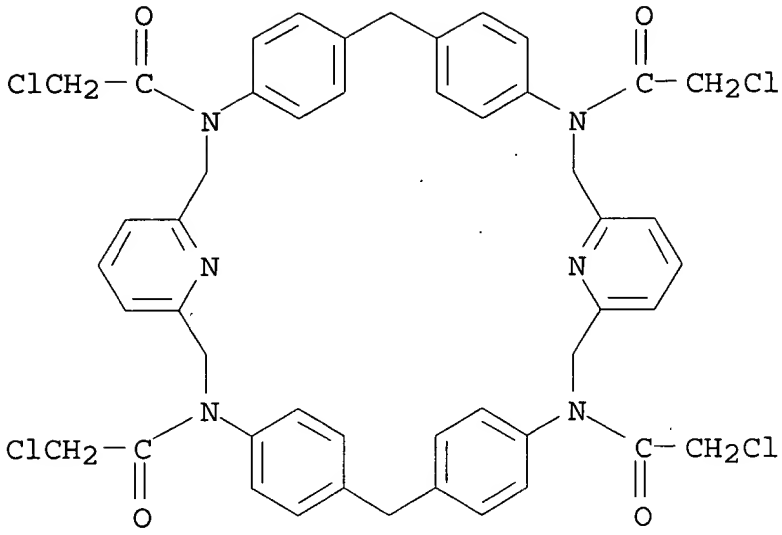
I

AB The synthesis of the new receptor I (R = COCH2N+Me3 Cl- contg. two pyridino and two diphenylmethane subunits is reported. It is remarkably sol. in water (up to 0.1 M) and can bind metal ions such as Cu(II) and org. mols. such as p-nitrophenol and 1,8-anilinonaphthalenesulfonic acid. The complexation const. for Cu(II) is rather modest, whereas the binding of the org. mols. is comparable to that of the other receptors such as cyclodextrins or other cyclophanes.

IT **118996-31-9P**
(prepn. and quaternization of, with trimethylamine)

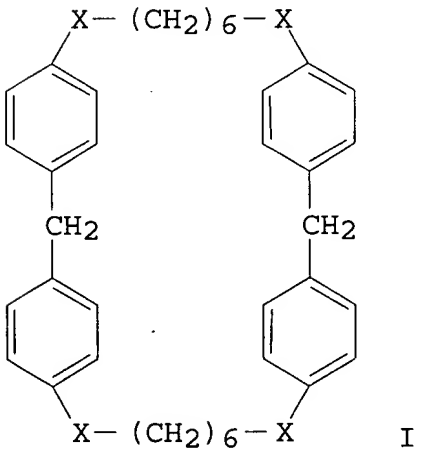
RN 118996-31-9 ZCA

CN 7,15,25,33,39,44-Hexaazaheptacyclo[32.2.2.23,6.216,19.221,24.19,13.127,31]hexatetraconta-3,5,9,11,13(44),16,18,21,23,27,29,31(39),34,36,37,40,42,45-octadecaene, 7,15,25,33-tetrakis(chloroacetyl)- (9CI) (CA INDEX NAME)



IT **118996-31-9P**
(prepn. and quaternization of, with trimethylamine)

L13 ANSWER 25 OF 27 ZCA COPYRIGHT 2003 ACS
110:7596 Host-guest chemistry. 19. Modification of hydrophobic and polar reciprocal interaction by charged groups in host-guest complexes. Schneider, Hans Joerg; Blatter, Thomas (Inst. Org. Chem., Univ. Saarlandes, Saarbruecken, D-6600/11, Fed. Rep. Ger.). Angewandte Chemie, 100(9), 1211-12 (German) 1988. CODEN: ANCEAD. ISSN: 0044-8249. OTHER SOURCES: CASREACT 110:7596.
GI



I

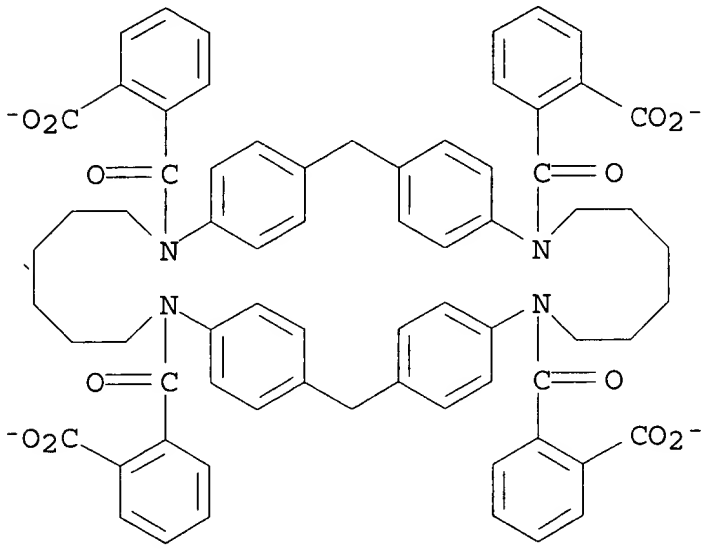
AB The formation consts. and complexation free energies for the complexes between the prepd. diphenylmethane-derived

tetraazacyclophanes I (X = m-NSO2C6H4SO3-, o-NCOC6H4CO2-, N+Me2) and 1-C10H7R (R = H, NH2, N+Me3Cl-) and 2-C10H7SO3- were detd. by NMR and related to the noncovalent interactions in the complexes.

IT **116405-69-7P**
(prepn., conformation, and interaction of, with naphthalene guests)

RN 116405-69-7 ZCA

CN Benzoic acid, 2,2',2'',2'''-(7,14,24,31-tetraazapentacyclo[30.2.2.23,6.215,18.220,23]dotetraconta-3,5,15,17,20,22,32,34,35,36,37,38-dodecaene-7,14,24,31-tetrayltetracarbonyl)tetrakis-, ion(4-) (9CI) (CA INDEX NAME)



IT **116405-69-7P**
(prepn., conformation, and interaction of, with naphthalene guests)

L13 ANSWER 26 OF 27 ZCA COPYRIGHT 2003 ACS

103:195708 Selective functionalization of hydrocarbons. 6. Mechanistic and preparative studies on the regio- and stereoselective paraffin hydroxylation with peracids. Schneider, Hans Joerg; Mueller, Walter (Univ. Saarlandes, Saarbruecken, D-6600/11, Fed. Rep. Ger.). Journal of Organic Chemistry, 50(23), 4609-15 (English) 1985. CODEN: JOCEAH. ISSN: 0022-3263. OTHER SOURCES: CASREACT 103:195708.

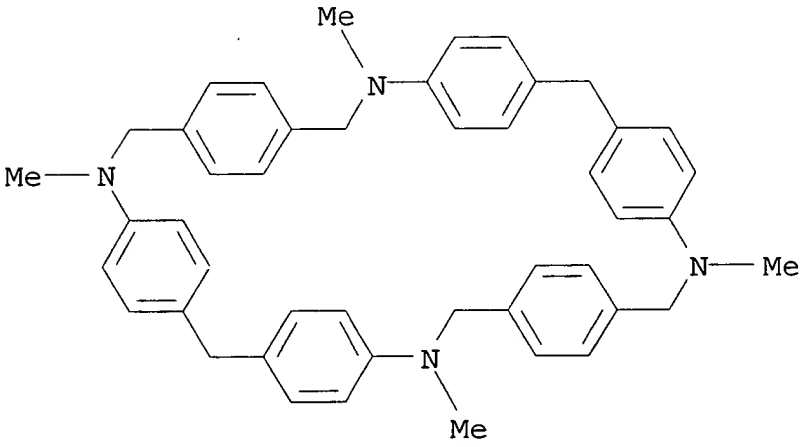
AB Reactions of >20 hydrocarbons with, e.g., p-nitro- or 3,5-dinitroperbenzoic acid in CHCl3 show regioselectivities of 90-500 (relative rates of attack at tertiary and secondary C-H bonds, after statistical correction) and configurational retention, if applicable, of 97-99.7%. Radical side reactions are responsible for a decrease in regio- and stereoselectivity. Steric effects are obsd. in attack at axial tertiary C-H bonds and at bridgehead positions. Electroneg. and H-bonding substituents in the alkane diminish, and alkyl groups enhance the rates; the Taft .delta.*

value of -2.2 indicates substantial pos.-charge accumulation in the transition state, in agreement with the high regioselectivity. A Hammett reaction const. of 0.63 is obtained from substituted perbenzoic acids; activation parameters of .DELTA.H* = 15-19 kcal/mol and .DELTA.S* = -22 to -29 e.u. with 3 alkanes of different flexibility and an isotope effect of kH/kD = 2.2 with methylcyclohexane are measured. Arom. rings are usually not attacked, but lead to peracid deactivation even at remote alkane C-H positions; similar deactivation is found in H-bonding solvents. Androstanes yield preferentially 9.alpha.- and 5.alpha.-hydroxy products, if, e.g., a 17.beta.-acetoxy substituent is used to steer the reaction. Diols usually are only obsd. as a result of a proximity effect of a peracid assocd. at the 1st-formed OH group. The results point to relatively late and oxenoid transition states with substantial charge sepn. in the substrate.

IT **98634-01-6**
(reactions of)

RN 98634-01-6 ZCA

CN 7,14,24,31-Tetraazaheptacyclo[30.2.2.23,6.29,12.215,18.220,23.226,29]hexatetraconta-3,5,9,11,15,17,20,22,26,28,32,34,35,37,39,41,43,45-octadecaene, 7,14,24,31-tetramethyl- (9CI) (CA INDEX NAME)



IT **98634-01-6**
(reactions of)

L13 ANSWER 27 OF 27 ZCA COPYRIGHT 2003 ACS

101:229575 Selective functionalizations of hydrocarbons. V. Regio- and stereoselectivity of the radical chlorination of cycloalkanes with different halogen carriers and host-guest complexes. Schneider, Hans Joerg; Philippi, Klaus (Fachrichtung Org. Chem., Univ. Saarlandes, Saarbruecken, D-6600/11, Fed. Rep. Ger.). Chemische Berichte, 117(10), 3056-74 (German) 1984. CODEN: CHBEAM. ISSN: 0009-2940. OTHER SOURCES: CASREACT 101:229575.

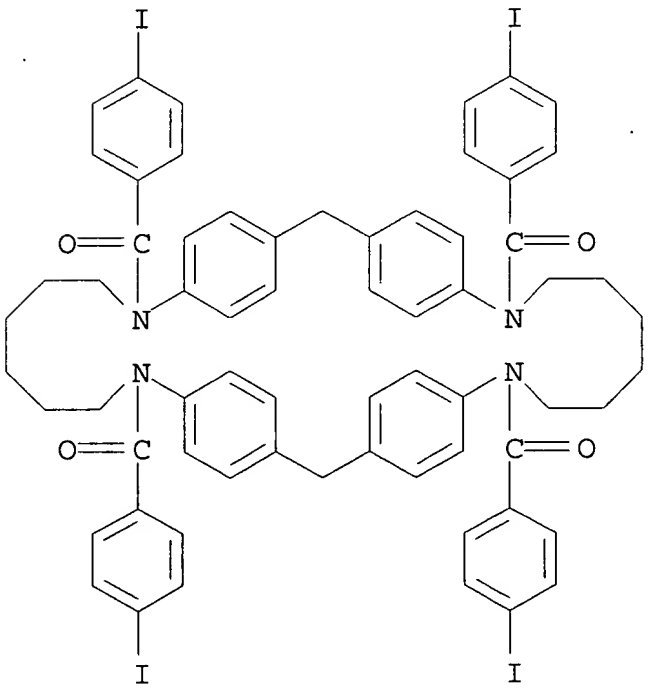
AB The reaction of trans-1,4-dimethylcyclohexane with PhICl2 (I), with most para-substituted I, and with Cl2 in CS2 shows a regioselectivity of Rst .simeq. 10; reactions with ortho-substituted

I or with I in HOAc or H2O show appreciable conversion, but lower sensitivities of Rst .simeq. 5. Tertiary cyclohexyl radicals are chlorinated preferentially from the axial side with I; ortho-substituents in I, or replacement of CCl4 by CS2 or benzene lead to lower stereoselectivities. Chlorinations with iodophenyl derivs. bound to a steroid matrix exhibit no significant change in regioselectivity; the same is obsd. for reactions with chlorine in the presence of newly synthesized macrocyclic azacyclophane salts in water, although these form inclusion complexes with the hydrocarbons used and inhibit the hydrolysis of chlorides from Tetralin. .alpha.-Cyclodextrin, however, leads by selective complexation to selective chlorination of the primary C-H bonds. Syntheses and 13C NMR shifts of the azacyclophanes are described.

IT **93367-97-6P**
(prepn. of)

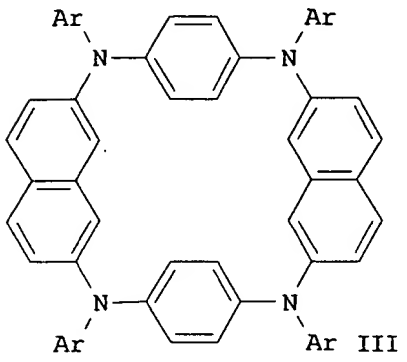
RN 93367-97-6 ZCA

CN 7,14,24,31-Tetraazapentacyclo[30.2.2.23,6.215,18.220,23]dotetraconta-3,5,15,17,20,22,32,34,35,37,39,41-dodecaene, 7,14,24,31-tetrakis(4-iodobenzoyl)- (9CI) (CA INDEX NAME)

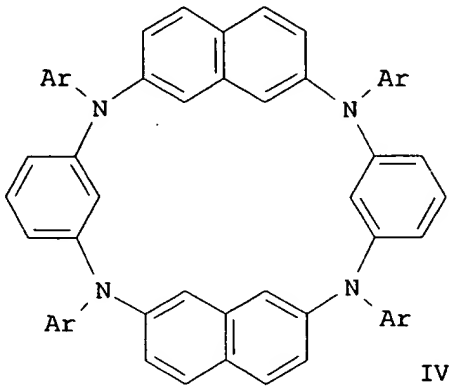


IT **93367-97-6P**
(prepn. of)

L12 ANSWER 4 OF 6 CAPLUS COPYRIGHT 2002 ACS
AN 1999:699801 CAPLUS
DN 132:35427
TI Macrocyclic Poly Arylamines for Rigid Connection of Poly Radical Cation Spins
AU Selby, Trent D.; Blackstock, Silas C.
CS Department of Chemistry, The University of Alabama, Tuscaloosa, AL, 35487-0336, USA
SO Org. Lett. (1999), 1(13), 2053-2055
CODEN: ORLEF7; ISSN: 1523-7060
PB American Chemical Society
DT Journal
LA English
GI



III



IV

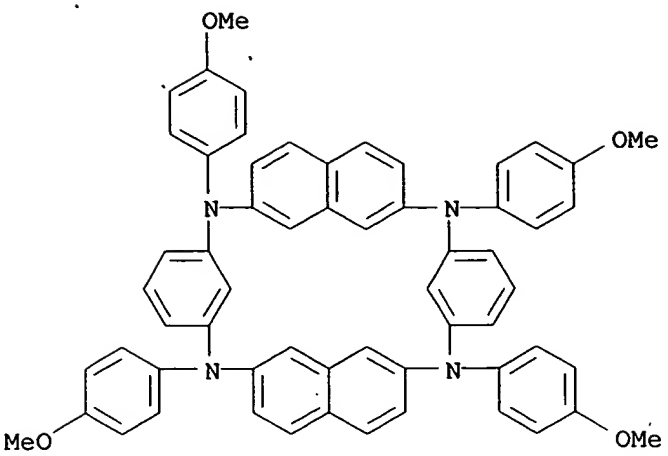
AB The synthesis of macrocyclic arylamines 3 and 4 (III and IV; Ar = 4-MeOC6H4) is reported. These structures yield conformationally rigid polyradical cations for investigation of their electron spin properties. Dication 32+ has dual N and N' connection of its p-phenylenediamine radical cation units via 2,7-naphthalene bridges. By ESR and NMR anal., 32+ is found to possess a populated, low-lying triplet excited state. Macrocycle 4 undergoes multielectron oxidn. as obsd. by cyclic voltammetry to yield polycations with more limited kinetic stability. Authors advise caution in handling shock-sensitive explosive thianthrenium perchlorate.

IT **252255-25-7 252255-27-9 252256-62-5**
RL: FMU (Formation, unclassified); PRP (Properties); FORM (Formation, nonpreparative)
(ESR and NMR magnetic susceptibility study of thermally populated low-lying triplet excited state of a conformationally rigid macrocyclic poly arylamine dication)

RN 252255-25-7 CAPLUS
CN 2,7-(Imino[1,3]benzenimino[2,7]naphthalenimino[1,3]benzenimino)naphthalene, 9,16,25,32-tetrakis(4-methoxyphenyl)-, radical ion(1+), perchlorate (9CI) (CA INDEX NAME)

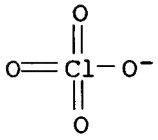
CM 1

CRN 252255-24-6
CMF C60 H48 N4 O4
CCI RIS
CDES 8:RI,(1+)



CM 2

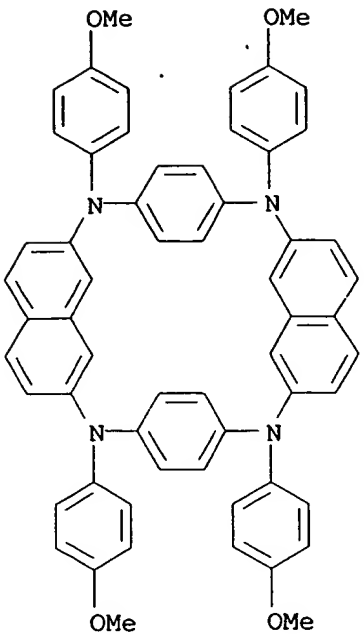
CRN 14797-73-0
CMF Cl O4



RN 252255-27-9 CAPLUS
CN 2,7-(Imino[1,4]benzenimino[2,7]naphthalenimino[1,4]benzenimino)naphthalene, 9,16,25,32-tetrakis(4-methoxyphenyl)-, radical ion(1+), perchlorate (9CI) (CA INDEX NAME)

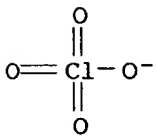
CM 1

CRN 252255-26-8
CMF C60 H48 N4 O4
CCI RIS
CDES 8:RI,(1+)



CM 2

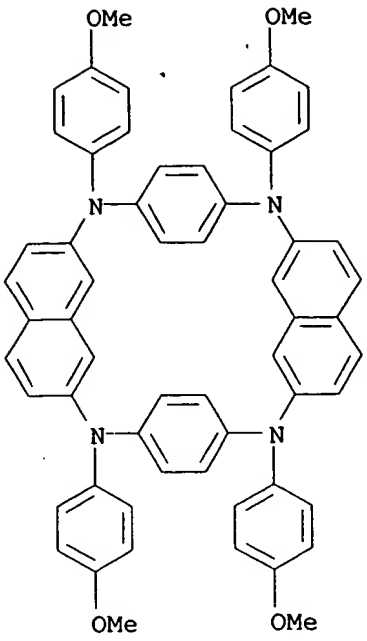
CRN 14797-73-0
CMF Cl O4



RN 252256-62-5 CAPLUS
CN 2,7-(Imino[1,4]benzenimino[2,7]naphthalenimino[1,4]benzenimino)naphthalene, 9,16,25,32-tetrakis(4-methoxyphenyl)-, radical ion(2+), diperchlorate (9CI) (CA INDEX NAME)

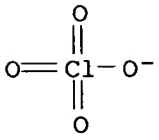
CM 1

CRN 252256-61-4
CMF C60 H48 N4 O4
CCI RIS
CDES 8:RI,(2+)

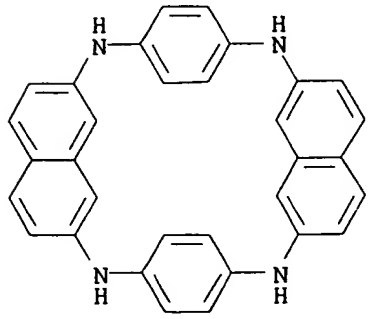


CM 2

CRN 14797-73-0
CMF Cl O4



IT **252255-23-5**
RL: PRP (Properties)
(conformation as model compd.; ESR and NMR magnetic susceptibility study of thermally populated low-lying triplet excited state of a conformationally rigid macrocyclic poly arylamine dication)
RN 252255-23-5 CAPLUS
CN 2,7-(Imino[1,4]benzenimino[2,7]naphthalenimino[1,4]benzenimino)naphthalene (9CI) (CA INDEX NAME)



IT **252255-22-4P**
RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)
(crystallog.; ESR and NMR magnetic susceptibility study of thermally

populated low-lying triplet excited state of a conformationally rigid macrocyclic poly arylamine dication)

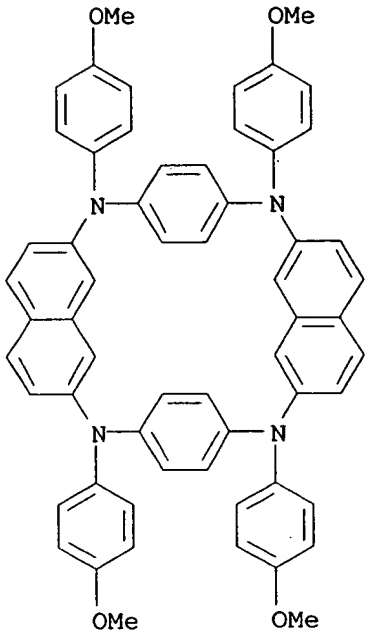
RN 252255-22-4 CAPLUS

CN 2,7-(Imino[1,4]benzenimino[2,7]naphthalenimino[1,4]benzenimino)naphthalene, 9,16,25,32-tetrakis(4-methoxyphenyl)-, compd. with nitrobenzene (1:1) (9CI) (CA INDEX NAME)

CM 1

CRN 252255-19-9

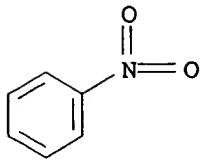
CMF C60 H48 N4 O4



CM 2

CRN 98-95-3

CMF C6 H5 N O2



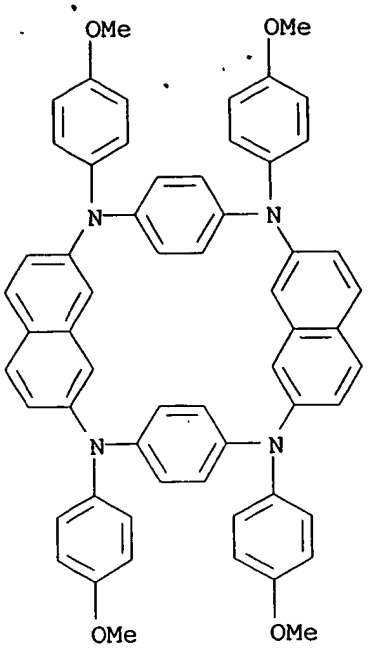
IT **252255-19-9P 252255-20-2P**

RL: PRP (Properties); RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation)

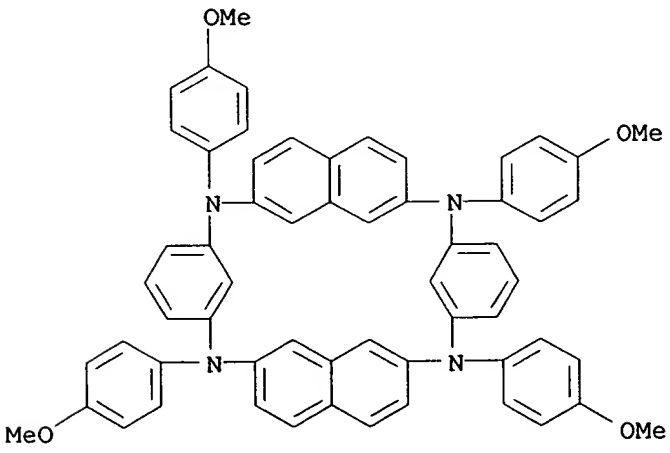
(electrooxidn. and chem. oxidn.; ESR and NMR magnetic susceptibility study of thermally populated low-lying triplet excited state of a conformationally rigid macrocyclic poly arylamine dication)

RN 252255-19-9 CAPLUS

CN 2,7-(Imino[1,4]benzenimino[2,7]naphthalenimino[1,4]benzenimino)naphthalene, 9,16,25,32-tetrakis(4-methoxyphenyl)- (9CI) (CA INDEX NAME)



RN 252255-20-2 CAPLUS
CN 2,7-(Imino[1,3]benzenimino[2,7]naphthalenimino[1,3]benzenimino)naphthalene
, 9,16,25,32-tetrakis(4-methoxyphenyl)- (9CI) (CA INDEX NAME)



RE.CNT 15 THERE ARE 15 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT